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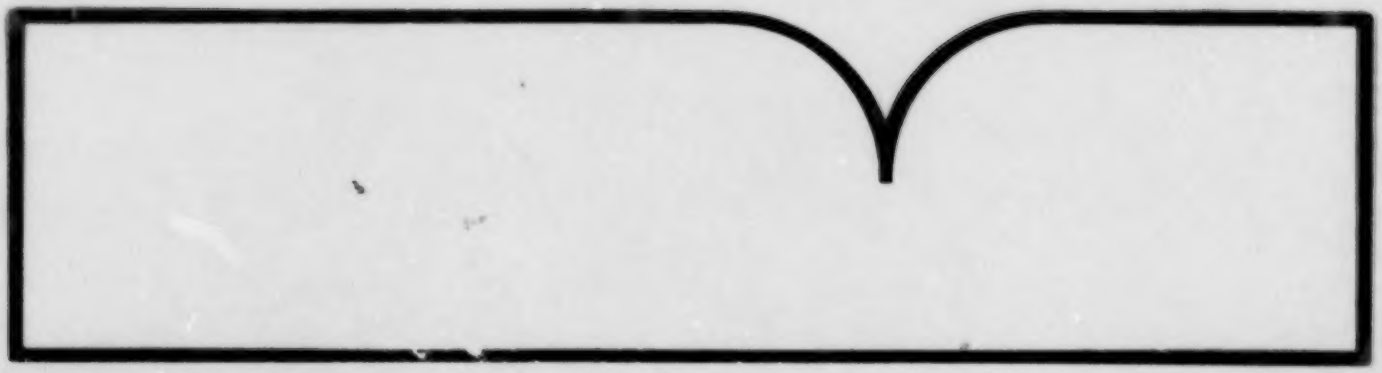
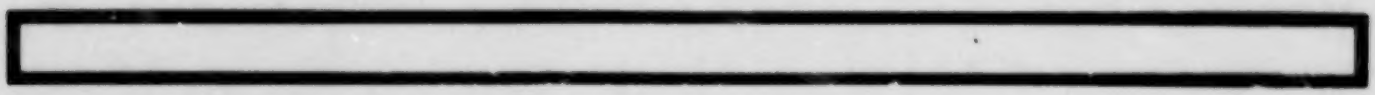
Exposure Analysis Modeling System
Reference Manual for EXAMS 2

(U.S.) Environmental Research Lab., Athens, GA

May 85





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16. ABSTRACT

The Exposure Analysis Modeling System (EXAMS), published in 1982 (EPA-600/3-82-023), provides rapid evaluations of the behavior of synthetic organic chemicals in aquatic ecosystems. EXAMS combines laboratory data describing reactivity and thermodynamic properties of chemicals with independent data describing the transport and physical/chemical properties of aquatic ecosystems. From these data, EXAMS computes exposure, fate and persistence. This manual describes the expansion of EXAMS to extend the model's capabilities to include seasonal differences in the environmental driving forces that govern transport and transformation kinetics, to compute the fate and transport of products that result from transformation reactions in the environment, and to provide greater flexibility in specifying the timing and duration of chemical loadings entering the ecosystem. Among other improvements, EXAMS II expands the treatment of ionic speciation and sorption to include trivalent ions, and complexation with "dissolved" organic matter. The suite of output tables has been expanded to accommodate product chemistry, pulse loadings, and other new input data and to provide analogous outputs for all operational modes.

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E X P O S U R E A N A L Y S I S M O D E L I N G S Y S T E M

Reference Manual for EXAMS II

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FOREWORD

Environmental protection efforts are increasingly directed toward preventing adverse health and ecological effects associated with specific compounds of natural or human origin. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Environmental Systems Branch studies complexes of environmental processes that control the transport, transformation, degradation, fate, and impact of pollutants or other materials in soil and water and develops models for assessing exposures to chemical contaminants.

Concern about environmental exposure to synthetic organic chemicals has increased the need for techniques to predict the behavior of chemicals entering the environment as a result of the manufacture, use, and disposal of commercial products. The Exposure Analysis Modeling System (EXAMS), which has been undergoing development, test, and revision at this Laboratory since 1978, provides a convenient tool to aid in judging the environmental consequences should a specific chemical contaminant enter a natural aquatic system. Because EXAMS requires no chemical monitoring data, it can be used for new chemicals not yet introduced into commerce as well as for those whose pattern and volume of use are known. EXAMS and other exposure assessment models should contribute significantly to efforts to anticipate potential problems associated with environmental pollutants.

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P R E F A C E

The first version of the EXAMS computer code concentrated on the long term results of continual, steady discharges of single chemicals into typical aquatic systems. Comments and requests from users (notably EPA's Office of Pesticide Programs and Office of Toxic Substances) have led to expansions of EXAMS' capabilities to:

1. include seasonal differences in the environmental driving forces that govern transport and transformation kinetics,

2. compute the fate and transport of products that result from transformation reactions in the environment, and to

3. provide greater flexibility in specifying the timing and duration of chemical loadings entering the ecosystem.

These objectives were implemented as follows.

1. Seasonal effects were added to EXAMS by expanding the environmental data to allow for 12 (monthly) entries, plus an average value at sector 13 of the database. The average values can be specified directly, or computed from the monthly data, as a user option. To simplify data aquisition, EXAMS II estimates some quantities that EXAMS I requires as input data. Most importantly, EXAMS II generates the solar light field from meteorological data. This algorithm is based on results from the research group led by A.E.S. Green at the University of Florida. From the latitude and elevation of the location, plus (monthly) data on atmospheric ozone, air mass types, atmospheric turbidity, and relative humidity, EXAMS computes 46 values of (clear-sky, 24-h average) photon flux density (photons/s/cm2/N nm where N is the bandwidth) covering the solar spectrum from 280 to 800 nm.

2. Transformation products are computed for each spatial and temporal (monthly) segment defined by the analyst. The program uses information describing the (temperature-dependent) mole/mole yield of product(s) from each of nine reaction processes (direct photolysis, etc.). The yields are further separated according to ionic speciation (up to seven species) and according to physical separation into dissolved, complexed (with "dissolved" organic matter), sediment-sorbed, and biosorbed forms (the latter for metabolic transformation processes only). The code checks for mass balance closure (i.e., it detects attempted transformations in excess of the available parent materials), and generates autochthonous chemical

loadings of the product chemicals. The fate and transport of the products are computed from process data held in the chemical database, that is, the behavior of daughter compounds is simulated in the same way as are the parent chemical(s).

3. EXAMS II includes two time-varying operational modes, in addition to the (Mode 1) steady-state capabilities implemented in EXAMS I. In Mode 2 operations, the user is ceded command of the integrator timer controls, and thus can evaluate the transport and fate of chemicals via initial-value problem approaches. Both steady chemical loadings and/or pulse loads (i.e., initial conditions) can be imposed on each spatial segment. A RUN command then invokes an integration package to simulate chemical behavior over the user-chosen interval. A "CONTINUE" command lets the user evaluate intermediate results, modify chemical loadings or environmental conditions, and re-invoke the integrator for additional sequenced simulations. Mode 3 simulations return control of the integrator to EXAMS, but give the user automated access to the entire suite of time-varying (monthly) environmental parameters. In Mode 3 operations, a suite of steady loadings can be set to vary on a monthly basis and, in addition, a chemical pulse can be loaded into any segment on any day (or series of days) of the year. In this way, complex load patterns due to the vagaries of manufacturing schedules and weather conditions can be accommodated. A Mode 3 "RUN" encompasses a minimum of one year, with no explicit maximum. During Mode 3 operations, EXAMS reports the 24-h, 96-h, and chronic exposure concentrations experienced in the system, as well as a sensitivity analysis reflecting the non-linear (i.e., second-order) nature of the governing equations. The integrators used in EXAMS II are double precision, variable-order variable-stepsize codes employing Adams methods upon initial invocation, followed (when necessary) by invocation of a "Gear's method" backward differentiation code for problems diagnosed as stiff.

There are additional differences between the EXAMS I and EXAMS II codes: The treatment of ionic speciation and sorption has been expanded to include trivalent ions and complexation with "dissolved" organic matter. EXAMS now computes the concentration of singlet oxygen in the water column, and the chemical database accepts rate constants for this transformation process. Reductive transformations have been included as a (provisional) second-order empirical equation. Oxidizing radicals are now entered as single near-surface values, and the code computes segment concentrations from light extinction in the ulra-violet. The suite of output tables has been expanded to include a description of ionic speciation, to accomodate the new input data (product chemistry, pulse loadings), and to provide analogous outputs for all operational modes. The physical geometry of the system can now be specified in several alternative ways -- for example, EXAMS II can accept the length, width, and mean depth of a reach, and itself compute segment volumes, etc.

A B S T R A C T

The Exposure Analysis Modeling System (EXAMS), published in 1982 (EPA-600/3-82-023) provides rapid evaluations of the behavior of synthetic organic chemicals in aquatic ecosystems. EXAMS combines laboratory data describing reactivity and thermodynamic properties of chemicals with independent data describing the transport and physical/chemical properties of aquatic ecosystems. From these data, EXAMS computes:

1) Exposure: the expected (long-term chronic, 24-hour and 96-hour acute) environmental concentrations due to a user-specified pattern of chemical loadings,

2) Fate: the distribution of the chemical in the system and the relative dominance of each transport and transformation process, and

3) Persistence: the time required for effective purification of the system (via export/transformation processes) once the chemical loadings terminate (in evaluative Mode 1 analyses).

EXAMS is an interactive program; it allows a user to specify and store the properties of chemicals and ecosystems, modify the characteristics of either via simple English-like commands, and conduct an efficient, rapid series of evaluations and sensitivity analyses that help the analyst discern the probable aquatic fate and effects of synthetic organic chemicals.

This manual describes the expansion of the EXAMS code to extend its capabilities to include seasonal differences in the environmental driving forces that govern transport and transformation kinetics, to compute the fate and transport of products that result from transformation reactions in the environment, and to provide greater flexibility in specifying the timing and duration of chemical loadings entering the ecosystem. Among other improvements, EXAMS II expands the treatment of ionic speciation and sorption to include trivalent ions, and complexation with "dissolved" organic matter. The suite of output tables has been expanded to accommodate product chemistry, pulse loadings, and other new input data and to provide analogous outputs for all operational modes.

This report covers a period from January 30, 1981 to April 15, 1985, and work was completed as of April 15, 1985.

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EXAMS Command Language User's Guide

This section describes the EXAMS command language, including usage and reference information. The first part of the Section provides an overview of the command language and its grammar. The second part contains detailed descriptions of each command. The commands are listed in alphabetical order.

Conventions used in this Section:

Convention	Meaning
CTRL/x	The phrase CTRL/x indicates that you must press the key labeled CTRL while you simultaneously press another key, for example, CTRL/O.
EXAMS > LIST 7 . . .	Vertical series of periods, or ellipsis, mean that not all the data EXAMS would display in response to the particular command is shown, or that not all the data a user would enter is shown.
keyword,...	Horizontal ellipsis indicates that additional keywords, command parameters, or data can be entered in a command sequence, or that EXAMS displays additional data as part of the sample output line.
[keyword]	Square brackets indicate that the item enclosed is optional, that is, the entity can be omitted from the command line altogether.

Overview:

The EXAMS command language provides users with a set of commands for:

- Entering, storing, and manipulating data describing the reaction chemistry of synthetic compounds, the environmental parameters governing their transport and fate in aquatic systems, patterns of allochthonous loadings, and product chemistry.
- Studying the results of an analysis by listing tabular output on your terminal, plotting the concentration data ("Expected Environmental Concentrations" or EECs) computed during simulations, and printing paper copy for later reference.

- Choosing an analytical framework for investigating exposure to chemicals in a particular case study: EXAMS includes three operational modalities or "MODEs":

MODE	Analytical Methodology
1	Long-term consequences of continued releases of chemicals; steady-state analysis.
2	Detailed examination of immediate consequences of chemical releases; initial-value problems.
3	Intermediate-scale resolution of events over several years, including effects of seasonal environmental variablity; analysis of time-series data.

Entering Commands

EXAMS commands consist of English-language words (usually verbs) that describe what you want EXAMS to do. Some commands include options that modify their operation. They provide EXAMS with more information on how you want the command to be executed. Some commands require a description of the object to be acted on by the command. In some cases, the object is a keyword (as in the HELP command); sometimes it is an EXAMS data element (SET command), or a section of a file of input data or analysis results (STORE and LIST commands).

Throughout this section, EXAMS commands are printed in uppercase letters. You can, however, enter these commands in uppercase, lowercase, or a mixture of uppercase and lowercase letters.

The following example shows an AUDIT command and EXAMS' response, as they would appear on your terminal:

```
EXAMS > AUDIT ON

All input will now be copied into the file
named AUDOUT.DAT on Fortran unit number  4

EXAMS > ! This Command File should be renamed file.EXA

FXAMS >
```

EXAMS analyzes the parts of the above example as follows.

EXAMS > The EXAMS system prompt for command input; a greater-than (>) means that EXAMS' command interpreter is ready for you to enter a command.

AUDIT — The command name, requesting that EXAMS enable/disable the User Notepad/Command File Creation facility.

ON — An option of the AUDIT command, requesting that the Notepad/Create facility be enabled.

```
All input will now be copied into the file
named AUDOUT.DAT on Fortran unit number  4
```

A message from the AUDIT command, indicating that the command completed sucessfully. The command interpreter used the value of AUDOUT (4) to establish communication with an external file.

EXAMS > — The next system command prompt, confirming that the command has completed its operations (AUDIT has opened communications with an external file and started recording terminal inputs), and EXAMS is ready for additional input.

! This Command File should be renamed file.EXA
A comment. A comment line always begins with an exclamation point (!) or an asterisk (*). You can use comments, as needed, to document EXAMS analysis sessions or command procedures.

EXAMS > — The next EXAMS system command prompt, confirming that the comment has been recorded in the Notepad/Command file and EXAMS is ready to accept another command.

Command Prompting

When you enter a command at the terminal, you need not enter the entire command on a single line. If you enter a command that requires that you specify its range or the object of the requested action, and you do not include the needed information, EXAMS' command interpreter prompts you for all missing information. For example:

```
EXAMS > AUDIT

The following AUDIT options are available:

        ON   - invokes the AUDIT option
        OFF  - terminates the AUDIT option
        HELP - this message
        EXIT - return to the EXAMS prompt.

AUDIT > ON

All input will now be copied into the file
named AUDOUT.DAT on Fortran unit number  4
```

In this example, no AUDIT option was entered, so EXAMS prompts for a more complete specification of the intended action. The line ending with a > indicates that EXAMS is waiting for the additional input.

In many cases, EXAMS' prompts do not include an automatic description of the full range of possible response options. Often, however, entering HELP in response to the prompt will display a list of available choices, as the following example indicates:

```
EXAMS > LIST

 Table > HELP

  1 Chemical inputs:  FATE Data
  2 Chemical inputs:  PRODUCT Chemistry
  3 PULSE Chemical Loadings
     .
     .
     .
 20 Exposure Analysis SUMMARY
ALL Entire Report

 Table > 18
Ecosystem: Name of Waterbody
Chemical:  Name of chemical
------------------------------------------------------------
TABLE 18.01.  Analysis of steady-state fate ...
------------------------------------------------------------
    .
    .  (body of table)
    .
------------------------------------------------------------
```

In the example above, LIST is entered without the number of the output table to be displayed. EXAMS prompts for the missing information; typing HELP in response to the LIST prompt displays a catalog of the available result tables.

EXAMS Messages

When you enter a command incorrectly, EXAMS' command interpreter will display a descriptive error message telling you what was wrong. For example, if you specify a data subscript larger that the maximum currently available on your machine, EXAMS will respond:

```
Subscript out-of-range.
```

You must then retype the command correctly.

Other error messages may be produced during the execution of a command, or during a simulation or data display sequence. These messages can indicate such things as incomplete environmental data, character data entered where

numeric data is required, or typographic errors during entry of commands. EXAMS will respond to typographic errors in command entries by displaying:

```
Command not recognized.  Type HELP for command information.
```

Because the messages are descriptive, you can usually determine what corrective action is required in order to proceed. When this is not the case, EXAMS' HELP facility contains a large body of additional and supplementary information available through the HELP, DESCRIBE, and SHOW commands.

The HELP Command

You may not always have this guide available at your terminal when you need a summary of the syntax of a command or a definition of an input datum. The HELP command provides this information in EXAMS' interactive environment. For example, you can type the command:

```
EXAMS > HELP LIST
```

EXAMS responds by displaying a description of the LIST command, its syntax, and the options you enter to specify the range of the command.

The HELP facility also provides on-line assistance for EXAMS' input data:

```
EXAMS > HELP QUANT
```

will display the subscript ranges, their meanings, the physical dimensions, and the English definition of EXAMS chemical input datum "QUANT". This information is available online for all EXAMS' input data and control parameters. The names of all of EXAMS' input variables have been selected as mnemonics for their English-language names. (For example, QUANT is the photochemical quantum yield.) These mnemonics are used in EXAMS' output tables; definitions are given in the Glossary of this User Manual.

EXAMS' Help facility supplies lists of individual topics and subtopics. The HELP command is described in more detail later in this Section, and a tutorial explanation of the command is available online by entering:

```
EXAMS > HELP TUTOR
```

Command Procedures

A command procedure is a file that contains a sequence of EXAMS commands, optionally interspersed with descriptive comments (lines with "!" or "*" in column one). By placing sets of frequently-used commands and/or response options in a command procedure, you can execute all the commands in it with a single command. For example, suppose a file called START.EXA contains these command lines and comments:

```
SET MODE TO 3
SET KCHEM TO 4
SET NYEAR TO 5
RECALL LOAD 7
! Load UDB Sector 7 is the spray vector study
```

You can execute the four commands in this file by entering the command:

```
EXAMS > DO START
```

or `EXAMS > @START`

You do not have to specify the file type of a command procedure when you use the @ command, so long as the file type is EXA. This is the default file type for EXAMS' @ command. You can use another file suffix, if you so inform EXAMS when you enter the command request. For example, to execute commands in a file named START.UP:

```
EXAMS > @START.UP
```

Wild Card Characters

Some EXAMS commands accept a "wild card" character in their input command specifications. The asterisk (*) is the only symbol having this function in EXAMS. Wild card characters are used to refer to a range of data subscripts, or other entities, by a general name, rather than having to enter a specific name for each member of the group. Particular uses of wild cards in EXAMS vary with the individual commands. The command descriptions later in this Section indicate where wild cards are allowed and their effects.

Truncating Command Names and Keywords

All keywords and names of input data that you enter as command input can be abbreviated. You need enter only enough characters to distinguish a keyword or datum from others with similar names.

Summary Description of EXAMS' System Commands

EXAMS Command	Summary Description
AUDIT	Start/Stop user notepad for recording procedures
CATALOG	List the contents of User Databases (UDBs)
CHANGE/SET	Enter/reset input data and program controls
CONTINUE	Resume integration (Modes 2 and 3 only)
DESCRIBE	Report dimensions and data type of parameter

DO or @	Execute file of EXAMS commands (file.EXA)
ERASE	Clear section of stored database (UDB)
EXIT/QUIT	Abort command, or End interactive session
HELP	Describes access to EXAMS on-line HELP facility
LIST	Show tabular results on the screen
NAME	Specify the name of a UDB, e.g., CHEM NAME IS ...
PLOT	Plot results on the screen
PRINT	Queue tabular results for hardcopy printing
RECALL	Activate data from stored database (UDB)
RUN	Begin simulation run
SHOW	Display current data values or control settings
STORE	Download current data into stored database (UDB)
ZERO	Clear chemical loadings, pulses, or residuals

A U D I T

Creates a copy of user input commands and responses in an external file.

Related: Control variables: AUDOUT
Commands: DO

Syntax: AUDIT option

Options

ON
OFF

Prompt: The following AUDIT options are available:

ON - invokes the AUDIT option
OFF - terminates the AUDIT option
HELP - this message.
EXIT - return to the EXAMS prompt.

AUDIT >

Options: OFF

Ends copying of EXAMS commands to the external file.

ON

Begins copying of EXAMS commands to an external file.

Description: The AUDIT command initiates copying of inputs typed at the terminal, into an external file. These inputs include EXAMS commands, and user responses to EXAMS prompts and option selections. The output terminus for the copy is a file named "AUDOUT.DAT," connected to Fortran logical unit number AUDOUT. AUDOUT can be modified (using the SET command) to any appropriate integer. The resulting output file can be used to record an analysis procedure, or as a general notepad. The output file can be renamed "file.EXA" and used as an EXAMS command (DO) file.

Examples:

1. EXAMS > AUDIT

The following AUDIT options are available:

```
                    ON   - invokes the AUDIT option
                    OFF  - terminates the AUDIT option
                    HELP - this message.
                    EXIT - return to the EXAMS prompt.

AUDIT > ON

All input will now be copied into the file
named AUDOUT.DAT on Fortran unit number  4
```

This command begins recording of terminal input in an external file. The output will go to a disk file named "AUDOUT.DAT." After leaving EXAMS, this file can be printed to give a permanent record of the analysis.

2. `EXAMS > AUDIT OFF`

```
The AUDIT option has been terminated.
```

This command ends copying of EXAMS commands and responses to the external medium (usually a disk file).

3. `EXAMS > AUDIT ON`

```
All input will now be copied into the file
named AUDOUT.DAT on Fortran unit number  4

EXAMS > RECALL ENV 2

Selected environment is: Phantom Inlet

EXAMS > RECALL CHEM 2

Selected compound is: Dichloromucktane

EXAMS > RECALL CHEM 4 AS 2

Selected compound is: Tetrabromochickenwire

EXAMS > AUDIT OFF
```

These commands build a file (AUDOUT.DAT) that can later be used as a command file upon entering the EXAMS system. In this instance, the file would be renamed (e.g., COMND.EXA) and used to execute the above series of commands as a unit:

```
EXAMS > DO COMND
```

C A T A L O G

Lists, by access number, the title of all currently active entries in the specified User Database (UDB).

Related: Control variables: none
Commands: ERASE, NAME, RECALL, STORE

Syntax: CATALOG option

Options

CHEMICAL
ENVIRONMENT
LOAD
PRODUCT

Prompt: Enter ENVIRONMENT, CHEMICAL, LOAD, PRODUCT, HELP or EXIT >

Options: CHEMICAL

Lists the titles, by access number, of chemical databases currently in the User Database. Each entry corresponds to a single chemical, and contains the laboratory data describing ionization and (species-specific) partitioning and reaction kinetics.

ENVIRONMENT

List the titles, by access number, of environmental databases currently in the User Database. Each entry contains a canonical physical and chemical model of an aquatic system, including the environmental data needed to compute reactivity and transport of synthetic chemicals in the system.

LOAD

Lists the titles, by access number, of allochthonous chemical loading patterns stored in the User Database. These data include monthly values (kg/hour) for stream-loads, non-point-source loads, groundwater seepage loads, precipitation loads, and drift loads of chemicals entering the aquatic environment, plus specification of pulse loadings. The pulse load data include the magnitude (kg), target environmental segment, and scheduling (month and day) of pulses of synthetic chemicals entering the system.

PRODUCT

Lists the titles, by access number, of reaction or transformation product chemistries stored in the User

Database. These data include the Activity Database numbers of chemical parent and product compounds, the number of the process responsible for the transformation, and the yield efficiency (mole/mole) as an (optional) function of temperature.

Description: The CATALOG command inventories the contents of the specified User Database (UDB) and lists the titles of active entries on the terminal screen. Four types of UDBs are available, corresponding to the four options available to the CATALOG command. The titles are listed by access number. This number is used to STORE, RECALL, or ERASE database entries.

Examples:

1. EXAMS > CATALOG HELP

```
The CATALOG command supports the following options
        1. ENVIRONMENT,
        2. CHEMICAL,
        3. LOAD,
        4. PRODUCT,
        5. HELP (this option), or
        6. EXIT.

Enter ENVIRONMENT, CHEMICAL, LOAD, PRODUCT, HELP or EXIT >

CHEMICAL

Catalog of chemicals

No. CHEMICAL NAME
  1 Unspecified Chemical
  2 p-Cresol
  3 Benz[a]anthracene
  .
  .
  .

EXAMS >
```

This command lists the contents of the current User Database for chemical data. Any of these datasets can be loaded into the Activity Database (ADB) for study, using the RECALL command and the appropriate access number. The first entry ("Unspecified Chemical") is a template for entering new chemical data.

2. EXAMS > CATALOG ENVIRON

```
Catalog of environments
  No. ENVIRONMENT NAME
    1 Unspecified Environment
    2 Pond -- AERL code test data
    3 Oligotrophic lake -- AERL code test data
    4 Eutrophic lake -- AERL code test data
    5 River -- AERL code test data
    .
    .
    .

EXAMS >
```

This command generates a listing of the environmental datasets present in the User Database. Any of these can be recalled for study using a RECALL command and the access number. The first entry ("Unspecified Environment") is a template for entering a new environmental model.

C H A N G E

Used to specify the values of data in the activity database.

Related: Commands: DESCRIBE, HELP

Syntax: CHANGE variable TO value

Prompt: CHANGE (VARIABLE TO VALUE) >

Variable: The data entry or variable to be CHANGEd can be specified either as a single datum or, using wild cards (*), as an entire vector, row/column of a matrix, etc.

Description: Use the CHANGE command to specify the values of data in the activity database. "Value" can be any numerical quantity or literal, as appropriate. "Variable" specifies an individual element of input data or a program control parameter. Entire vectors, rows/columns of matrices, etc. can be set to single values using wild cards (*).

Examples:

1. EXAMS > CHANGE VOL(27) TO 7E5

   Subscript out-of-range.

   EXAMS > DESCRIBE VOL

   VOL is a Real Vector with 25 elements.

   EXAMS> CHANGE VOL(2) TO E

   Invalid numeric quantity after TO.

   EXAMS > CHANGE VOL(2) TO 7E5

   This command sets the environmental volume of segment 2 to 7.0E+05 cubic meters. The initial attempt to set the volume of segment 27 was rejected by EXAMS because the version in use was set up for environmental models of 25 segments at most. The DESCRIBE command was used to check the number of subscripts and the dimensional size of the variable "VOL". The erroneous

entry of an alphabetic for the volume was trapped by the CHANGE command; the initial value of VOL(2) was not altered.

2. EXAMS > HELP TCEL

TCEL is a Real Matrix with 25 rows and 13 columns.
Temperature-CELsius (segment,month) Units: degrees C.
Average temperature of ecosystem segments.
Used (as enabled by input data) to compute effects of temperature on transformation rates and other properties of chemicals.

EXAMS > CHANGE TCEL(2,7) TO 24

This command changes the July temperature in segment 2 to 24 degrees C. The HELP command was used to check subscript dimensions, maximum values, the meaning of the subscripts (subscript #1 denotes the segment, subscript #2, the month), and the proper units for the input datum (Celsius degrees).

3. EXAMS > HELP POH

POH is a Real Matrix with 25 rows and 13 columns.
pOH (segment,month) Units: pOH units
The negative value of the power to which 10 is raised in order to obtain the temporally averaged concentration of hydroxide [OH-] ions in gram-equivalents per liter.

EXAMS > CHANGE POH(*,13) TO 6.2

This command sets the average pOH (sector 13) of every segment to 6.2. Note use of wild card "*" to specify that all segments are to be changed. As in the previous example, HELP was used to check subscript dimensions, units, etc. This step, of course, is optional.

C O N T I N U E

The CONTINUE command resumes EXAMS' simulation analysis of chemical dynamics beginning from the current state of the system.

Related: Control variables: CINT, NYEAR
Commands: RUN, SHOW TIME FRAME

Syntax: CONTINUE

Prompt: (In Mode 2 only:)
Initial time for integration will be (nn.n) units
Enter ending time of integration, HELP, or EXIT >

Options: None. Reply to prompt with a value greater than (nn.n).

Description: The CONTINUE command resumes EXAMS' simulation analysis of chemical dynamics, beginning from the current state of the system. Chemical loadings and other input data can be altered (CHANGEd or SET) between simulation segments; EXAMS will re-evaluate equation parameters as needed to incorporate the changed conditions into the analysis.

CONTINUE cannot be invoked from Mode 1, where it is not appropriate. The SHOW TIME FRAME (abbreviate to SH TI F) command can be used to assess the current state of the integrator timer controls. In Mode 2, the Communications INTerval CINT can be used to vary the temporal resolution in different segments of the analysis (see Example 1). In Mode 3, NYEAR, the number of years in a simulation time segment, can be similarly varied.

Examples:

1. EXAMS > SET MODE=2

   EXAMS > SHOW TIME FRAME

   A RUN will integrate from 0. to 24. Hours
   with output at intervals of 2.00 Hours

   EXAMS > SET TCODE=2

   EXAMS > SET TEND=10

   EXAMS > SET CINT=0.25

   EXAMS > ST TI F

   A RUN will integrate from 0. to 10. Days
   with output at intervals of 0.25 Days

```
EXAMS > RUN

Simulation beginning for:
Environment:  Pond -- AERL code test data
Chemical  1:  Dichloromucktane

Run complete

EXAMS > PLOT KIN PL  (1,4,0,0 -- see PLOT command)

System:  Pond -- AERL code test data
Chemical:  Dichloromucktane
  2.00          IBB BBB
                I      B BBBB BBBB
                I                  BBBB BBBB BBB
                I                               B BBBB BBBB BB
                I                                             BB BBB
  1.33          I
                I
                I
                I
                I
  0.667         I
                I
                I
                I
                I
  0.000         I
                 +----+----+----+----+----+----+----+----+----+----+
                0.000      2.00       4.00       6.00       8.00       10.0
                     1.00       3.00       5.00       7.00       9.00
                                Time, Days

                EXAMS > SET CINT=1

                EXAMS > CONTINUE

                Initial time for integration will be                10.0 Days
                Enter ending time of integration, HELP, or EXIT > 30

                Simulation beginning for:
                Environment: Pond -- AERL code test data
                Chemical  1: Dichloromucktane

                Run complete.

                EXAMS > SET CINT=10

                EXAMS > ZERO PULSE LOAD

                EXAMS > CONTINUE
```

```
Initial time for integration will be                30.0 Days
Enter ending  time  of  integration,  HELP,  or  EXIT  >  90

Simulation beginning for:
Environment: Pond -- AERL code test data
Chemical  1: Dichloromucktane

Run complete.

EXAMS > PLOT KINETIC PLOT (1,4,0,0)

System:   Pond -- AERL code test data
Chemical: Dichloromucktane
  3.49     I      B
           I      BB
           I       BB
           I         B
           I          BB
  2.33     I            BB
           IB             BB
           IBBB             BBB
           I   BBB
           I     BB               B
  1.16     I                          B
           I                              B
           I                                   B    B     B
           I
           I
  0.000    I
            +----+----+----+----+----+----+----+----+----+----+
           0.000     18.0      36.0      54.0      72.0      90.0
                9.00      27.0      45.0      63.0      81.0
                                Time, Days
```

These commands show the use of the CONTINUE command in Mode 2. The objective of the analysis was to introduce two pulses of chemical separated by ten days and to follow exposure over 90 days. Note the phased increase in the Communications INTerval CINT from 0.25 to 1 and then 10 days. Note the use of the ZERO command to clear the pulse load ADB before the simulation of dissimilation from day 30 through day 90. If this were not done, EXAMS would introduce an additional pulse on day 30.

```
2.  EXAMS > SET MODE=3

    EXAMS > SHO TI FR

    A RUN will integrate from 1 January  1985
                        through 31 December 1985.
    (YEAR1 = 1985, and NYEAR =   1.)

    EXAMS > RUN
```

```
Simulation beginning for:
Environment: Pond -- AERL code test data
Chemical   1: Dichloromucktane

Run complete.

EXAMS > SHO TI FR

A RUN will integrate from  1 January  1985
                    through 31 December 1985.
(YEAR1 = 1985, and NYEAR =   1.)

CONTinuation will proceed through 31 December 1986
(NYEAR =    1.)

EXAMS > SET NYEAR=3

EXAMS > SH TI F

A RUN will integrate from  1 January  1985
                    through 31 December 1987.
(YEAR1 = 1985, and NYEAR =   3.)

CONTinuation will proceed through 31 December 1988
(NYEAR =    3.)

EXAMS > CONTINUE

CONTinuing integration through 31 December 1988.

Simulation beginning for:
Environment: Pond -- AERL code test data
Chemical  1: Dichloromucktane

Run complete.

EXAMS >
```

These commands illustrate the use of the CONTINUE command in Mode 3. SHOW TIME FRAME is used to assess the state of the integrator timer controls.

D E S C R I B E

Reports the data type, dimensionality, and implemented size of parameters.

Related: Control variables:
Commands: HELP

Syntax: DESCRIBE parameter

Parameters:

Any "system parameter" -- any chemical or environmental input datum, control parameter (e.g., MODE, CINT), etc.

Prompt: Enter SYSTEM PARAMETER name >

Options: Any parameter accessible to the CHANGE and SET commands can be inspected using the DESCRIBE command.

Description: The DESCRIBE command returns information about EXAMS' input data and control parameters. All variables whose values can be altered using the CHANGE and SET commands can be inspected by the DESCRIBE command. The information returned by DESCRIBE includes the data type (real, integer, character), dimensionality (scalar, vector, matrix (2-dimensional), table (3-dimensional matrix)) and implemented size in the version of EXAMS in use. The DESCRIBE command is the first recourse when a CHANGE or SET command fails.

Examples:

1. EXAMS > DESR MODE

Command not recognized. Type HELP for command information.

EXAMS > DESCR

Enter SYSTEM PARAMETER name > MODE

MODE is an Integer Scalar.

These commands establish that "MODE" is an integer scalar. Note that the initial typing error (DESR) resulted in a "not recognized" error message followed by return to the EXAMS prompt.

2. EXAMS > CHANGE VOL(27) TO 7E5

Subscript out-of-range.

EXAMS > DESCRIBE VOL

VOL is a Real Vector with 25 elements.

This command reports that VOL is a real variable, with 25 elements. In this example, the number of segments (NPX) in the version of EXAMS currently in use is set for 25 at most. Any (intentional or accidental) attempt to set "KOUNT" to a value >25, or to enter a value for the VOLume of a segment >25 (e.g., VOL(27)) will fail, as illustrated above. DESCRIBE can be used to check the reason for a failure of the CHANGE or SET command when a problem with dimension sizes is suspected.

3. EXAMS > DESCRIBE QUANT

QUANT is a Real Table with dimensions (3,7,4)

EXAMS > HELP QUANT

QUANT is a Real Table with dimensions (3,7,4)
QUANTum yield (form,ion,chemical) Units: dimensionless
Reaction quantum yield for direct photolysis of chemicals -- fraction of the total light quanta absorbed by a chemical that results in transformations. Separate values (21) for each potential molecular type of each chemical allow the effects of speciation and sorption on reactivity to be specified in detail. The matrix of 21 values specifies quantum yields for the (3) physical forms: (1) dissolved, (2) sediment-sorbed, and (3) DOC-complexed; of each of (7) possible chemical species: neutral molecules (1), cations (2-4), and anions (5-7). (QUANT is an efficiency.)

These commands report the data type and dimensionality of EXAMS' input "QUANT" (result of "DESCRIBE QUANT") and then report the meaning of the dimensions and the physical units of the variable (result of "HELP QUANT"). The local implementation of EXAMS used in this example has the capacity to simulate the behavior of no more than four chemicals simultaneously. Thus, QUANT was DESCRIBEd as consisting of a set of four matrices, each of (fixed) size (3,7).

D O

Executes a command procedure; requests that EXAMS read subsequent input from a specific file.

Related: Control variables:
Commands: AUDIT

Syntax: DO file-spec

Prompt: Enter filespec, HELP, or EXIT >

Parameters: file-spec

Specifies the file from which to read a series of EXAMS commands. If you do not specify a file type, the system uses a default file type of EXA. Wild cards are not allowed in the file specification.

Description: Use command procedures to catalog frequently used sequences of commands. An EXAMS command procedure can contain:

- Any valid EXAMS command. The command line can include all the necessary options and data to build a complete command (exception: kinetic plots).
- Parameters or response options for a specific command. When the currently executing command requires additional parameters, the next line of the command file is searched for apropriate input.
- Data. When the currently executing command requires numerical or character data entry, the next line of the command file is searched for input.
- Comment lines. Any line that contains an exclamation point (!) or asterisk (*) in column one is ignored by EXAMS' command interpreter. These lines can be used as needed to document the command procedure.

Command procedures must not contain a request to execute another command procedure. In other words, a DO file must not contain a DO (@) command: EXAMS' DO commands cannot be nested.

Command procedures can be contructed as external files using your favorite editor, or they can be contructed interactively through the EXAMS system command processor, as illustrated below. The default file type is .EXA, but files of any type (suffix) can be used if the entire file name is specified when entering the DO command.

Examples:

1. EXAMS > AUDIT ON

   All input will now be copied into the file
   named AUDOUT.DAT on Fortran unit number 4

   EXAMS > RECALL

   Enter ENVIRONMENT, CHEMICAL, LOAD, PRODUCT,
   HELP or EXIT > ENV

   Enter environment No. or EXIT > 2

   Selected environment is: Phantom Inlet

   EXAMS > RECALL CHEM 2

   Selected compound is: Dichloromucktane

   EXAMS > RECALL LOAD 2

   Selected load is: Aedes spray drift

   EXAMS > ! LOAD 2 is the Phantom Inlet salt marsh study

   EXAMS > SET KCHEM TO 2

   EXAMS > RECALL CHEM 4 AS 2

   Selected compound is: Tetrabromochickenwire

   EXAMS > AUDIT OFF

These commands build a file (AUDOUT.DAT) that can later be used as a command file upon entering the EXAMS system. In this instance, the file could be renamed (e.g., SETUP.EXA) and used to execute the above series of commands as a unit:

```
EXAMS > DO SETUP
```

or

```
EXAMS > @SETUP
```

The command file appears as follows:

```
RECALL
ENV
2
RECALL CHEM 2
RECALL LOAD 2
! LOAD 2 is the Phantom Inlet salt marsh study
```

```
SET KCHEM TO 2
RECALL CHEM 4 AS 2
AUDIT OFF
```

Note that command files that are constructed interactively will include "AUDIT OFF" as the final instruction. This can, of course, be removed by editing the file if it is undesirable.

2. EXAMS > DO

```
Enter filespec, HELP, or EXIT > HELP

The "DO" or "@" command provides a means of executing
stored EXAMS commands. In response to the prompt, enter
the name of the file that contains the stored commands. A
filename extension of .EXA is supplied if one is not
explicitly specified.

Enter filespec, HELP, or EXIT > AUDOUT.DAT

EXAMS/DO >  ! Audit trail of input sequence from EXAMS.
EXAMS/DO >  RECALL
Enter ENVIRONMENT, CHEMICAL, LOAD, PRODUCT, HELP or EXIT >
EXAMS/DO >  ENV
Enter environment No. or EXIT >
EXAMS/DO >  2

Selected environment is: Phantom Inlet
EXAMS/DO >  RECALL CHEM 2

Selected compound is: Dichloromucktane
EXAMS/DO >  RECALL LOAD 2

Selected load is: Aedes spray drift
EXAMS/DO >  ! LOAD 2 is the Phantom Inlet salt marsh study
EXAMS/DO >  SET KCHEM TO 2
EXAMS/DO >  RECALL CHEM 4 AS 2

Selected compound is: Tetrabromochickenwire
EXAMS/DO >  AUDIT OFF

The AUDIT option has been terminated.
```

This command requests execution of the command procedure constructed in Example 1 above. The default name (AUDOUT.DAT) was not altered, so the complete file specification was given to the DO command as the entry parameter. The DO file transfers a set of 2 chemicals, an environmental model, and a load pattern from the stored UDB to the ADB for further study and analysis.

E R A S E

Deletes, by access number, the data stored at a single sector of a User Database (UDB) library (chemical, environmental, loadings, product chemistry).

Related: Control variables:
Commands: CATALOG, RECALL, STORE

Syntax: ERASE option access-number

Options

CHEMICAL
ENVIRONMENT
LOAD
PRODUCT

Prompt: Enter ENVIRONMENT, CHEMICAL, LOAD, PRODUCT, HELP or EXIT >

Options: CHEMICAL

Deletes the contents, by entry access number, of chemical databases currently in the User Database. Each entry corresponds to a single chemical, and contains the laboratory data describing ionization and (species-specific) partitioning and reaction kinetics.

ENVIRONMENT

Deletes the contents, by entry access number, of environmental databases currently in the User Database. Each entry contains a canonical physical and chemical model of an aquatic system, including the environmental data needed to compute the reactivity and transport of synthetic chemicals in the system.

LOAD

Deletes the contents, by entry access number, of chemical loading patterns stored in the User Database. These data include monthly values (kg/hour) for streamloads, non-point-source loads, groundwater seepage loadings, precipitation loads, and drift loads of chemicals entering the aquatic environment, plus the magnitude (kg), target environmental sector, and scheduling (month and day) of chemical pulse loads.

PRODUCT

Deletes the contents, by entry access number, of chemical product data stored in the User Database (UDB). These data include the Activity Database numbers of reactants and products, the number code of the chemical process, and (mole/mole) yield efficiencies as an (optional) function of temperature.

Description: ERASE deletes the contents of a single sector of the specified User Database (UDB) library (chemical, environmental, loads, or product chemistry). The data to be deleted are selected by choosing the appropriate access number. (If you work in a mulit-user environment, be sure to avoid erasing others' data!)

Examples:

1. EXAMS > ERASE ENV 20

Environment 20 erased.

This command erases the data stored at Environmental UDB sector number twenty. The space is now available for storage of another dataset.

2. EXAMS > ERASE

Enter ENVIRONMENT, CHEMICAL, LOAD, PRODUCT, HELP or EXIT >

HELP

The ERASE command supports the following options

1. ENVIRONMENT,
2. CHEMICAL,
3. LOAD,
4. PRODUCT,
5. HELP (this option), or
6. EXIT.

Enter ENVIRONMENT, CHEMICAL, LOAD, PRODUCT, HELP or EXIT >

LOAD

Enter load No. or EXIT > 10

Load 10 erased.

This command erases the data stored at Loadings UDB sector number ten. The space is now available for another dataset.

E X I T

Use EXIT to abort a command in progress or to end an interactive session.

Related: Control variables:
Commands: QUIT

Syntax: EXIT

Prompt: None

Options: None

Description: The EXIT command terminates processing of the current command procedure. If EXIT is used in response to an EXAMS command option, control is returned to the EXAMS prompt command level. If EXIT is entered from the EXAMS prompt command level, control is returned to your computer's operating system.

Examples:

1. EXAMS > AUDIT

   The following AUDIT options are available:

   ```
   ON   - invokes the AUDIT option
   OFF  - terminates the AUDIT option
   HELP - this message.
   EXIT - return to the Exams prompt.
   ```

   ```
   AUDIT > EXIT

   EXAMS >
   ```

   This command terminates processing of the AUDIT command and returns control to the EXAMS prompt command level. The current status of AUDIT is not altered.

2. EXAMS > EXIT

   This command terminates an interactive EXAMS session.

H E L P

Displays, on the terminal, information available in EXAMS' help files. EXAMS provides descriptions of its commands, input data, control parameters, and general concepts and analysis procedures.

Related: Control variables:
Commands: DESCRIBE

Syntax: HELP [keyword]

Prompt: None

Keyword: Specifies a keyword or topic that indicates what information you want.

- None -- if HELP is typed with no keyword, EXAMS lists the keywords that you can specify to obtain information about other topics.
- Topic-name -- describes either a basic EXAMS command, an information page, or a "system parameter." System parameters include chemical and environmental input data, system control parameters (e.g., CINT), and parameters that control the current analysis (e.g., IMASS).

Ambiguous abbreviations result in a failure to achieve a match on the keyword, and an error message is displayed.

Description: The HELP command provides access to EXAMS' collection of on-line user aids and information texts. This material includes:

- Brief discussions of the syntax and function of each of EXAMS' command words (RECALL, RUN, etc.)
- Definitions, physical dimensions, and meanings of subscripts for EXAMS' chemical and environmental input data and control parameters.
- A series of information pages providing orientation to the concepts implemented in the EXAMS program, the range of capabilities and analyses that can be executed with the

program, and brief expositions on data structures and program control options.

Examples:

1. EXAMS > HELP

```
Available commands and information pages:
  .
  . HELP message text and list of command and information
  . topics
```

Issuing the HELP command without any keywords produces a list of the HELP topics available in EXAMS main command library.

If you type in one of the topics on the list, EXAMS will display a HELP message on that topic, and a list of subtopics (if there are any).

2. EXAMS > HELP QUOIT

```
No information available for this request.

EXAMS >
```

When you request information for a topic not in EXAMS' files, EXAMS displays a message to that effect and returns you to the EXAMS > prompt.

3. EXAMS > HELP QUANT

```
QUANT is a Real Table with dimensions(3,7,4)
QUANTum yield (form,ion,chemical)     Units: dimensionless
Reaction quantum yield for direct photolysis of chemicals
-- fraction of the total light quanta absorbed by a chemi-
cal that results in transformations. Separate values (21)
for each potential molecular type of each chemical allow
the effects of speciation and sorption on reactivity to
be specified in detail. The matrix of 21 values specifies
quantum yields for the (3) physical forms: (1) dissolved,
(2) sediment-sorbed, and (3) DOC-complexed; of each of (7)
possible chemical species: neutral molecules (1), cations
(2-4), and anions (5-7). (QUANT is an efficiency.)
```

You can request information about any input datum (chemical, environmental, control parameters, analysis parameters) acces-

sible to the CHANGE and SET commands. EXAMS then displays on the screen the characteristics of the variable (equivalent to the results of DESCRIBE), followed by a discussion of the variable that echoes the entry in the Glossary section of your EXAMS User Manual.

L I S T

Displays an EXAMS output table on your terminal.

Related: Control variables: FIXFIL
Commands: PLOT, PRINT

Syntax: LIST option

Options

table-#
ALL
HELP

Prompt: Table > option

Options: table-# specifies the number of an EXAMS output table to be displayed.

ALL
Sequential display of all current output tables.

HELP
Displays a list of titles of EXAMS output tables.

Description: The LIST command displays EXAMS' output tables at your terminal. When the LIST command displays output, you can control the display in several ways:

- To temporarily halt the output and resume it at the line where it was interrupted, use CTRL/S followed by CTRL/Q.
- To suppress the display but continue processing the LIST command, use CTRL/O. If you press CTRL/O again before the command terminates, output resumes at the current point in the processing of the LIST command.

When you request a primary table number (that is, an integer from 1 to 20) EXAMS displays the first table of that number present in the analysis file. If additional tables of that type are present in the file, EXAMS will display the first, and then search for more tables of that type and, if any are found, ask if you want to see them.

Examples:

1. EXAMS > LIST

A PRINT, LIST, or PLOT command was issued before executing a RUN. If results exist from a previous simulation, these can be accessed after issuing the command:

SET FIXFIL TO 1

```
EXAMS > SET FIXFIL TO 1

EXAMS > LIST

 Table > HELP

  1 Chemical inputs:  FATE Data
  2 Chemical inputs:  PRODUCT Chemistry
  3 PULSE Chemical Loadings
     .
     .
     .
 18 Sensitivity Analysis of Chemical FATE
 19 Summary TIME-TRACE of Chemical Concentrations
 20 Exposure Analysis SUMMARY
ALL Entire Report

 Table > 18
Ecosystem: Name of Waterbody
Chemical:  Name of chemical
-------------------------------------------------------------
TABLE 18.01.  Analysis of steady-state fate ...
-------------------------------------------------------------
     .
     .  (body of table)
     .
-------------------------------------------------------------
```

The LIST command requests that output Table 18 from an EXAMS results file be displayed on the terminal. For illustrative purposes, it was assumed that the user had left EXAMS and then returned to inspect Table 18 generated in the previous session.

2. EXAMS > LIST 20

```
Ecosystem: Name of Waterbody
Chemical:  Name of FIRST chemical
```

```
-----------------------------------------------------------
TABLE 20.01.  Exposure analysis summary: 1983--1985.
-----------------------------------------------------------
  .
  .  (body of table)
  .

More ? (Y/N/Q) > Y

Ecosystem: Name of Waterbody
Chemical:  Name of SECOND chemical
-----------------------------------------------------------
TABLE 20.02.  Exposure analysis summary: 1983--1985.
-----------------------------------------------------------
  .
  .  (body of table)
  .
```

In this example, EXAMS was used to investigate the behavior of two chemicals over a period of several years, using Mode 3 simulations. The analysis began with year 1983, and NYEAR was set to 3 to produce an analysis of the period 1983 through 1985. The LIST command requests that all versions of Table 20 in the analysis file be displayed, with a pause between each for inspection of the results. In the example, the analyst chose to examine the output for both chemicals. If the analysis is now CONTINUEd, the current set of tables will be replaced with new results. The PRINT command should be used to make copies of all intermediate results you want to save.

The sub-table numbers of EXAMS' output tables identify the ADB number of the chemical, the number of any ionic species (see SPFLG in the Glossary), and the month of the year, as follows.

Table	Sub-tables	Examples	Sub-table Meaning
1	1.cc.i	1.01.1	Table.chemical.ion
4-6, 8, 10,11,13	NN.mm	4.01 10.13	Table.month (13 = annual mean)
12	12.cc.mm	12.01.12	Table.chemical.month
14 (Mode 1/2)	14.cc	14.01	Table.chemical
14 (Mode 3)	14.cc.mm	14.01.12	Table.chemical.month
15-18,20	NN.cc	18.01 20.01	Table.chemical

N A M E

Use the NAME command to attach unique names to datasets.

Related: Control Variables: MCHEM
Commands: CATALOG, ERASE, STORE, RECALL

Syntax: <datatype> NAME IS aaa... (up to 50 characters)
where <datatype> can be CHEM, ENV, LOAD, or PRODUCT

Prompt: Options available are:

```
HELP                    - this message.
EXIT                    - return to EXAMS command mode.
<carriage return>       - this message
<any other response>    - considered to be a new name.

NAME >
```

<datatype>: EXAMS uses these four kinds of datasets:

1. CHEMICAL reactivity and partitioning,

2. ENVIRONMENTal physico/chemical parameters,

3. allochthonous chemical LOADings, and

4. PRODUCT chemistry for generating interconversions among multiple chemicals in an analysis

Description: The NAME command is used to associate unique names with datasets in the UDB. These names can be STOREd in the CATALOGs; they are printed in the headers of EXAMS' output tables. When naming CHEMICAL datasets, the ADB number of the chemical to be named is given by MCHEM; use "SET MCHEM TO n" before naming chemical dataset "n".

Examples:

1. EXAMS > CHEM NAME IS Tetrachlorochickenwire

The NAME command associates the name "Tetrachloro..." with the chemical data in the sector of the activity database (ADB) given by the current value of MCHEM. This name will be printed on all subsequent appropriate output tables, and it will be used as a title for the database if the STORE command is used to download the data into the User Database (UDB).

2. EXAMS > SET MCHEM = 2

EXAMS > CHEM NAME IS Dichloromucktane

The chemical name command always addresses the MCHEM sector of the chemical ADB, thus, this example names chemical number 2 to "Dichloro...".

3. EXAMS > ENVIR NAME IS Pogue Sound

This command names the current environmental dataset "Pogue Sound". The name will now appear on output tables, and remain with the dataset if it is downloaded to the UDB permanent files.

P L O T

Used to plot character graphics for the chemical state of the ecosystem.

Related: Control Variables: MCHEM
Commands: LIST, PRINT

Syntax: PLOT [Option1, Option2, Option3]

Options:

POINT
PROFILE
KINETIC

Prompt: The following options are available:

```
POINT   - Vertical concentration profile
PROFILE - Longitudinal concentration profile
KINETIC - List or plot kinetic outputs
HELP    - This message
EXIT    - Return to the EXAMS prompt

Option >
```

Plot options: POINT

"POINT" plots are generalized profiles of chemical concentrations. These also require selection of a variable to be displayed (total concentration, dissolved concentration, etc.) and a "statistical" class (average values, minima, or maxima).

PROFILE

"PROFILE" plots are longitudinal profiles of chemical concentrations. These require selection of a concentration variable (total concentration, dissolved concentration, etc.) and an environmental sector (water column or benthic sediments). The abscissa of the resulting plot is set up by increasing segment number, which in most cases should represent an upstream-downstream progression. When the aquatic model includes both longitudinal and vertical segmentation, each section of the plot begins at the air-water or water/benthic interface and proceeds vertically downward (the bars are presented along the abscissa).

KINETIC

"KINETIC" plots display the results of integration of the governing equations over the time spans selected for simulation. These plots also require selection of concentration variables and either particular segments, or summary "statistics," for display. The first numerical parameter selected is used as the abscissa for the plot; all further selections plot on the ordinate.

Description: Use the PLOT command to display results of the current analysis. Three kinds of character-graphic PLOTs are available on-line from EXAMS: POINT, PROFILE, and KINETIC. Each PLOT requires the specification of several options; these can either be entered on the system command line or entered in response to EXAMS' prompts. The available second- and third-level options are illustrated in the examples below. The results available to POINT and PROFILE plots depend on the Mode used in the simulation. In Mode 1, the outputs are steady-state concentrations. In Mode 2, the results are a snap-shot of concentrations as of the end of the current temporal simulation segment. In Mode 3, the results are time-averaged concentrations over the most recent temporal simulation segment of length NYEAR.

Examples:

1. EXAMS > PLOT POINT

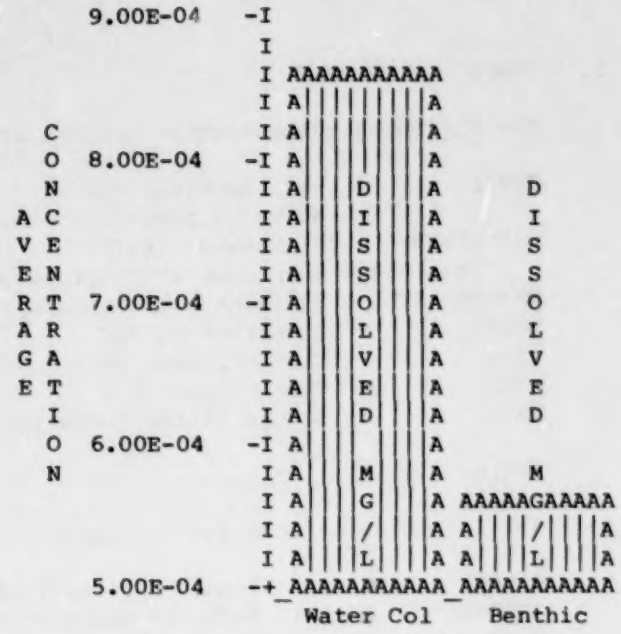
The following concentration options are available:

```
TOTAL       -  mg/L in Water Column,
               mg/kg in Benthic Sediments
DISSOLVED   - "Dissolved" (mg/L)
  (aqueous + complexes with "dissolved" organics)
PARTICULATE -  Sediment-sorbed (mg/kg)
BIOTA       -  Biosorbed (ug/g)
MASS        -  Chemical mass as grams/square meter AREA
HELP        -  This message
EXIT        -  Return to the EXAMS prompt

Option > DISSOLVED
```

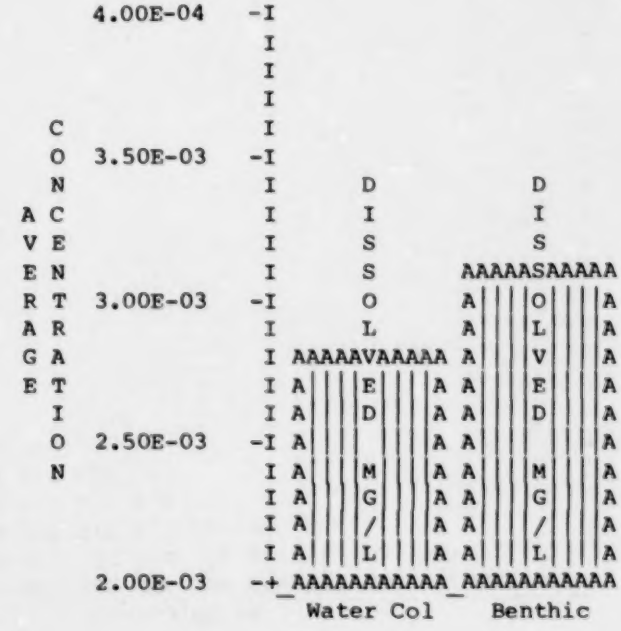
The following statistical options are available:

```
MAX    - Maximum concentration
MIN    - Minimum concentration
AVE    - Average concentration
MINMAX - For simultaneous plot of maxima and minima
HELP   - This message
EXIT   - Return to the EXAMS prompt
```

```
Option > AVERAGE
```

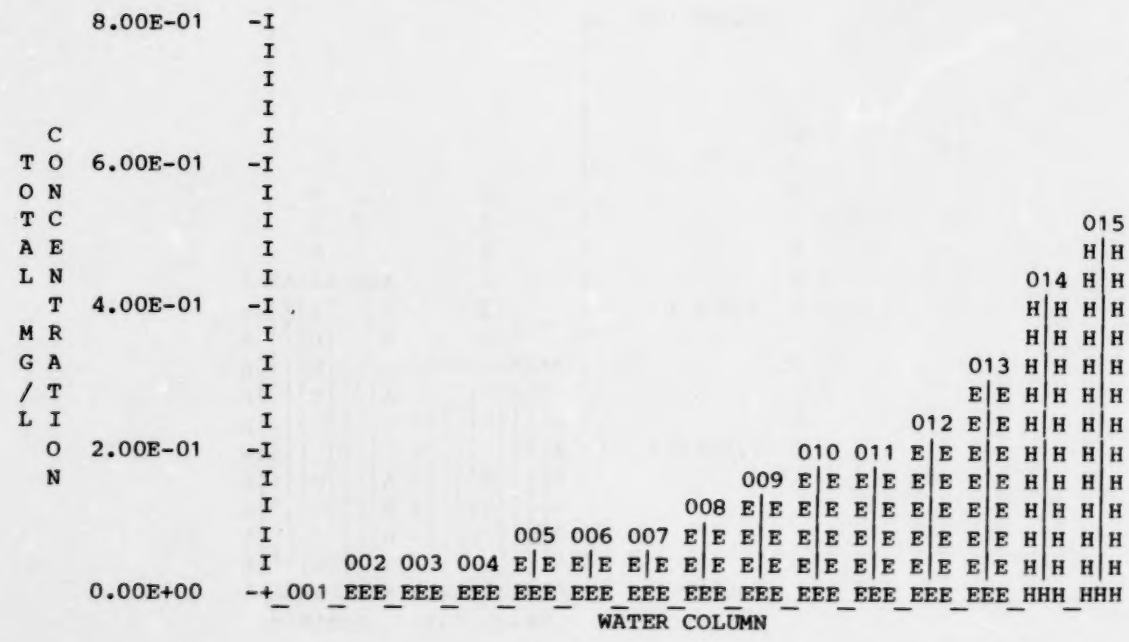



```
EXAMS > SET MCHEM=2

EXAMS > PL PO DI AV
```



This example illustrates EXAMS' internal prompting for POINT plots. Note that the analysis included two chemicals; the plot for chemical number two was obtained by first SETting MCHEM=2. The second plot was requested via a single command line, thus bypassing the PLOT prompts.

```
2.   EXAMS > PLOT PROF

     The following concentration options are available:

     TOTAL       -  mg/L in Water Column,
                    mg/kg in Benthic Sediments
     DISSOLVED   - "Dissolved" (mg/L)
         (aqueous + complexes with "dissolved" organics)
     PARTICULATE -  Sediment-sorbed (mg/kg)
     BIOTA       -  Biosorbed (ug/g)
     MASS        -  Chemical mass as grams/square meter AREA
     HELP        -  This message
     EXIT        -  Return to the EXAMS prompt

     Option > TOTAL

     The following options are available:

     WATER      - Water Column concentrations
     SEDIMENTS  - Benthic Sediment concentrations
     HELP       - This message
     EXIT       - Return to the EXAMS prompt

     Option > WATER
```



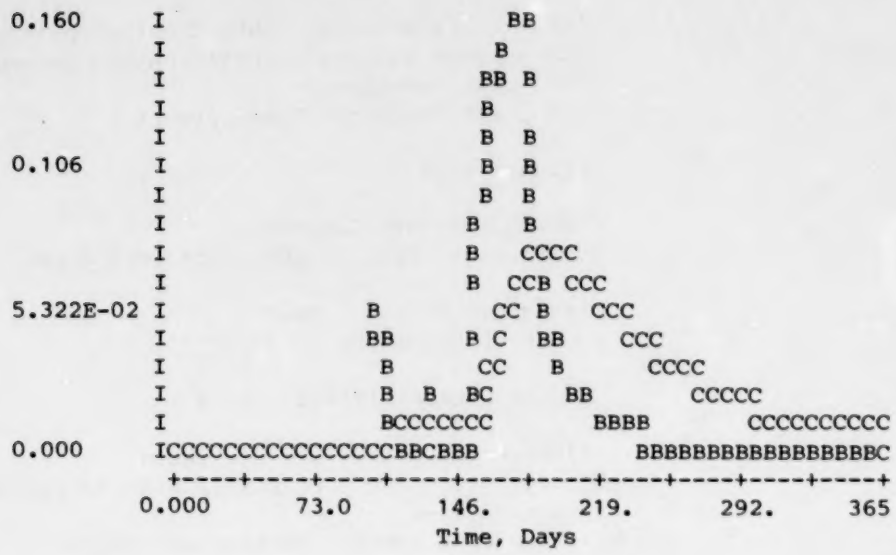
The above example illustrates EXAMS' internal prompts for a PROFILE plot. As with the POINT option, this entire command could be entered on a single line:

```
EXAMS > PLOT PROF TO WAT
```

3. `EXAMS > PLOT KIN`

```
The following KINETIC options are available:

LIST - lists selected KINETIC output parameters
PLOT - plots selected KINETIC output parameters
HELP - this message
EXIT - return to the EXAMS prompt

Option > PLOT

Chemical: Methyl Parathion
Environment: Pond -- AERL code test data

Simulation units:   Days
Number of segments:    2
                          1  2
Type of segment (TYPE):  L  B

The following parameters are available:
("Dissolved" = aqueous + complexes with "dissolved" organics.)
1 - Simulation time
2 - Water Column: average "dissolved" (mg/L)
3 -               average  sorbed    (mg/kg)
4 -               total mass         (kg)
5 - Benthic:      average "dissolved" (mg/L)
6                 average  sorbed    (mg/kg)
7                 total mass         (kg)

Enter parameters, one per line;
enter 0 to end data entry and proceed.

Parameter > 1
Parameter > 4
Parameter > 7
Parameter > 0


The following parameters are available for each segment:

1 -  Total concentration (Water Column, mg/L; benthic, mg/kg)
2 - "Dissolved"          (mg/liter of fluid volume)
3 -  Sorbed              (mg/kg of sediment)
4 -  Biosorbed           (ug/g)
5 -  Mass                (grams/square meter of AREA)
```

```
Enter segment-parameter number pair, one number per line;
enter 0 when data entry is complete; EXIT to abort.


Enter segment number   > 0


System:   Monthly pond -- AERL code test data
Chemical: Methyl Parathion

```




```
This example illustrates EXAMS' prompting in KINETIC  plots.
The numerical options cannot be entered on the command line,
but must be entered in response to the prompts.
```

P R I N T

Use the PRINT command to queue an output table for hardcopy printing.

Related: Control variables: FIXFIL
Commands: LIST

Syntax: PRINT option

Options:

table-#
ALL
HELP

Prompt: Table >

Options: table-# specifies the number of an EXAMS output table to be displayed.

ALL
Sequential printing of all current output tables.

HELP
Displays a list of titles of EXAMS output tables.

Description: The PRINT command transfers EXAMS results tables to an output queue for printing. The command functions identically with the LIST command, except that output is saved for hardcopy printing rather than being routed to your interactive terminal. If the PRINT command results in output at your terminal, you may need to consult with site ADP personnel to properly direct the print stream to a lineprinter.

Examples: See the documentation for the LIST command.

Q U I T

Use QUIT to end an interactive EXAMS session.

Related: Control variables:
Commands: EXIT

Syntax: QUIT

Prompt: None

Options: None

Description: Enter QUIT at the EXAMS prompt command level in order to terminate the interactive session. Control is returned to your computer's operating system.

Examples:

1. EXAMS > QUIT

This command terminates an interactive EXAMS session.

R E C A L L

Use RECALL to upload data from the permanent database (UDB) into current foreground memory (ADB).

Related: Control Variables: MCHEM

Commands: CATALOG, ERASE, NAME, STORE

Syntax: RECALL <datatype> UDB# [AS ADB#]

Prompt: Enter ENVIRONMENT, CHEMICAL, LOAD, PRODUCT, HELP or EXIT >

Command parameters:

<datatype> can be CHEMICAL, ENVIRONMENT, LOAD, or PRODUCT (EXAMS uses these four kinds of datasets.)

AS ADB# is an optional explicit specification of MCHEM (see Example 1).

UDB# specifies the accession number or location in the User Database for the source data for transfer to the ADB (Example 2).

Description: RECALL transfers data from permanent storage (UDBs) to activity databases (ADBs). The data in active use by EXAMS are held in a foreground memory bank (Activity DataBase or ADB) with four sectors, one for each datatype required by EXAMS:

CHEMICAL reactivity and partitioning,

ENVIRONMENTal physico/chemical parameters,

allochthonous chemical LOADings, and

PRODUCT chemistry for generating interconversions among multiple chemicals in an analysis.

When EXAMS is started, the ADB is empty. Use the RECALL command to transfer data from the permanent User Databases (UDBs) to foreground memory (ADB).

When an analysis session is ended (QUIT or EXIT), ADBs are discarded. Use the STORE command to transfer new data from the ADB to the UDB sector of the same datatype for permanent retention of the data.

Examples:

1. Because EXAMS can process several chemicals in a single analysis, the target sector of the chemical activity database should be specified when using the RECALL command to activate CHEMICAL data. (This section of the command should be omitted for other data types.) When the ADB# (an integer between 1 and KCHEM) is omitted, the chemical data is transferred to the sector of the activity database given by the current value of MCHEM. For example, to activate data from the chemical UDB, putting UDB dataset number 9 into ADB sector 1, and UDB #14 into sector 2:

Either:

```
EXAMS > SET MCHEM TO 1

EXAMS > RECALL CHEMICAL 9

EXAMS > SET MCHEM TO 2

EXAMS > RECALL CHEMICAL 14
```

or, equivalently:

```
EXAMS > RECALL CHEMICAL 9 AS 1

EXAMS > RECALL CHEMICAL 14 AS 2
```

2. Long-term retention of data required by EXAMS is provided by storage in the "User Database" (UDB, generally resident on a physical device--e.g., a hard disk) for CHEMICALs, ENVIRONMENTs, LOADs, or PRODUCTs. Within each of these UDB sectors, each dataset is CATALOGed via a unique accession number (UDB#). When transferring data to foreground memory (the activity database or ADB) from a UDB, the source location must be specified by the name of the UDB sector and the accession number within the sector. For example, to RECALL an environmental dataset:

```
EXAMS > RECALL ENVIR 2

Selected environment is:  Phantom Inlet, Bogue Sound

EXAMS >
```

R U N

The RUN command begins a simulation analysis.

Related: Control Variables: MODE
Commands: CONTINUE

Syntax: RUN

Prompt: None

Description: The RUN command executes an analysis and creates the output files accessed by the LIST and PLOT commands. The activity database (ADB) must be loaded, either via entry of new data or by RECALL from the UDB, before a RUN can be initiated.

Examples: 1.

```
EXAMS > RECALL CHEMICAL 22

Selected compound is: Dibromomucktane

EXAMS > RECALL ENVIRON 17

Selected environment is: Albemarle Sound - Bogue Bank

EXAMS > SET STRL(1,1,13)=.01

EXAMS > RUN

Simulation beginning for:
Environment: Albemarle Sound - Bogue Bank
Chemical  1: Dibromomucktane

Run complete.

EXAMS >
```

In this example, a steady-state (MODE=1) analysis is conducted by selecting a chemical and an environment, imposing a chemical loading of chemical 1 on segment 1 under average conditions (i.e., data sector 13, EXAMS initial default value) and invoking EXAMS simulation models with the RUN command.

S E T

Used to specify the values of data in the activity database.

Related: Commands: CHANGE (synonym), DESCRIBE, HELP

Syntax:
SET variable TO value
or
SET variable = value

Prompt: CHANGE (VARIABLE TO VALUE) >

Variable: The data entry or variable to be SET can be specified either as a single datum or, using wild cards (*), as an entire vector, row/column of a matrix, etc.

Description: Use the SET command to specify the values of data in the activity database. "Value" can be any numerical quantity or literal, as appropriate. "Variable" specifies an individual element of input data or a program control parameter. Entire vectors, rows/columns of matrices, etc. can be set to single values using wild cards (*).

Examples:

1.
```
EXAMS > SET VOL(27) TO 7E5

Subscript out-of-range.

EXAMS > DESCRIBE VOL

VOL is a Real Vector with 25 elements.

EXAMS> SET VOL(2) TO F

Invalid numeric quantity after TO.

EXAMS > SET VOL(2) TO 7E5
```

This command sets the environmental volume of segment 2 to 7.0E+05 cubic meters. The initial attempt to set the volume of segment 27 was rejected by EXAMS because the version in use was set up for environmental models of 25 segments at most. The DESCRIBE command was used to check the number of subscripts and

the dimensional size of the variable "VOL". The erroneous entry of an alphabetic for the volume was trapped by the SET command; the initial value of VOL(2) was not altered.

2. EXAMS > HELP TCEL

TCEL is a Real Matrix with 25 rows and 13 columns.
Temperature-CELsius (segment,month) Units: degrees C.
Average temperature of ecosystem segments.
Used (as enabled by input data) to compute effects of temperature on transformation rates and other properties of chemicals.

EXAMS > SET TCEL(2,7)=24

This command changes the July temperature in segment 2 to 24 degrees C. The HELP command was used to check subscript dimensions, maximum values, the meaning of the subscripts (subscript #1 denotes the segment, subscript #2, the month), and the proper units for the input datum (Celsius degrees).

3. EXAMS > HELP POH

POH is a Real Matrix with 25 rows and 13 columns.
pOH (segment,month) Units: pOH units
The negative value of the power to which 10 is raised in order to obtain the temporally averaged concentration of hydroxide [OH-] ions in gram-molecules per liter.

EXAMS > SET POH(*,13) TO 6.2

This command sets the average pOH (sector 13) of every segment to 6.2. Note use of wild card "*" to specify that all segments are to be changed. As in the previous example, HELP was used to check subscript dimensions, units, etc. This step, of course, is optional.

S H O W

Use SHOW to display current data values or control settings.

Related: Control Variables: MCHEM, MONTH

Commands: CHANGE, SET

Syntax: SHOW option [range]

Prompt: The following options are available:

Advection,	Chemistry,	Geometry,	Globals,
Loads,	Plot,	Pulse Loads,	Products
Quality,	Time Frame,	Turbulence,	Variables
HELP, or	EXIT >		

Command parameters:

Range: Some options of the SHOW command accept the specification of a range of values to define the scope of the data to be displayed (see Example 1). Use MCHEM to delimit the range of SHOW Chemistry, and MONTH for Geometry, Quality, etc.

Options:

ADVECTION

SHOW ADVECTION gives the advective hydraulic flow structure of the current aquatic system. A single element in a dataset might typically look like:

J_FR_AD	1	J_FRom_ADvection: Source Segment
I_TO_AD	3	I_TO___ADvection: Terminus
ADV_PR	1.00	ADVection_Proportion: Percent of total JFRAD flow on path
Path No.:	1	Vector index for SETting data

No more than NCON hydrologic pathways can be specified. If more are needed, this number can be increased and EXAMS recompiled. Specify export pathways by entering a zero (0) for the number of the segment to receive the flow (ITOAD). Do not specify a hydrologic source term by entering zero in the JFRAD vector; instead use streamflows, non-point-source flows, etc.

CHEMISTRY

SHOW CHEMISTRY displays the chemical output data currently in the ADB (foreground memory bank). The sector of the ADB denoted by the current value of MCHEM is displayed. Within each sector of the ADB (that is, for each chemical under active review), the data for each ionic species are presented separately, and photochemical data are presented on separate screens.

GEOMETRY

SHOW GEOMETRY returns a segment-by-segment description of the geometry (volumes, areas, etc.) of the current ecosystem. The segment number reported with each block of data is the first subscript for modifying the datum using CHANGE or SET. The month to be displayed is set by the current value of MONTH (explicit mean values are denoted by MONTH number 13): the month is the second subscript of such data as WIND, STFLD, etc.

GLOBALS

SHOW GLOBALS displays the input data that are "global" in extent, that is, "global" data apply to all segments of the current ecosystem.

LOADS

SHOW LOADS displays the current state of allochthonous chemical loadings. The form of the display depends on the current operational MODE: initial values are ignored in Mode 1 as they have no effect on the analysis results. The value of PRSW also affects the display: when PRSW is 0, SHOW LOADS returns a summary of annual loadings; when PRSW=1, a month-by-month tabulation is displayed as well. This display may not represent the final values used in the analysis, because EXAMS will modify loads that result in violation of the linearizing assumptions used to construct the program. After a RUN has been executed, however, SHOW LOADS will display the corrected values.

PRODUCTS

SHOW PRODUCTS displays the specifications for product chemistry currently in the ADB. Each entry is identified and loaded according to a unique "pathway number." A single element of a dataset might look like this:

CH_PAR	1	ADB number of CHemical PARent
T_PROD	2	ADB number of Transformation PRODuct

```
N_PROC          7     Number of transforming PROCess
R_FORM         29     Reactive FORM (dissolved, etc.)
YIELD M/M   0.100     Mole/Mole YIELD of product
EaYLD Kcal  0.000     Enthalpy of yield (if appropriate)
 Pathway:       1     Number of the pathway
```

More detail as to the numbering of NPROC and RFORM is given in the Glossary, and can be accessed via the HELP command. No more than NTRAN transformation pathways can be specified. If more are needed, this parameter can be increased and EXAMS recompiled.

PLOT

SHOW PLOT examines the contents of the concentration time-series and steady-state files, and reports the names of the chemicals and ecosystem used in the analysis.

PULSE LOADS

SHOW PULSE LOADS displays the specifications for allochthonous pulses of chemicals entering the system. This display may not represent the final values used in the analysis, because EXAMS will modify loads that result in violation of the linearizing assumptions used to construct the program. Although faulty pulse loads are discarded, EXAMS does not correct the input pulse load data, because the occurrence of load constraint violations depends on the context (i.e., the magnitude of current stream loadings, etc.). Thus, unlike SHOW LOADS, the SHOW PULSE display following execution of a RUN does not display corrected data. The pulses actually used during an analysis are instead displayed in EXAMS' output tables, where they can be examined using the LIST command.

QUALITY

SHOW QUALITY returns a segment-by-segment display of the canonical water-quality data included in the current ENVironmental ADB dataset. The month to be displayed is set by the current value of MONTH (explicit mean values are denoted by MONTH number 13). The month is the second subscript of such data as pH, pOH, etc. The first subscript is the segment number; thus these data are entered (CHANGE/SET) as "datum(segment,month)".

TIME FRAME

SHOW TIME FRAME displays the current status of the parameters needed to control the temporal aspects of a Mode 2 or Mode 3 simulation.

TURBULENCE

SHOW TURBULENCE displays the input data describing dispersive transport in the active (loaded in the ADB) ENVIRONMENTal dataset. The index vectors (JTURB, ITURB) define the existence of inter-segment dispersive transport paths. A zero in either vector, when paired with a non-zero value at the corresponding position in the other index vector, is taken as a boundary condition with an uncontaminated body of water. A single element in a dataset might typically be displayed like this:

```
J_TURB          1          Segment number for dispersion
I_TURB          2          Segment number for dispersion
XS_TUR m2   5.000E+04      Cross-sectional area of path
CHARL m       2.53         CHARacteristic_Length of path
DSP m2/hr   4.676E-05      Eddy DiSPersion coefficient
 Path No.:      1          Vector index for data entry
```

No more than NCON hydrologic pathways can be specified. If more are needed, this number can be increased and EXAMS recompiled.

VARIABLES

SHOW VARIABLES displays a list of the names of EXAMS input data and control parameters. These names must be used to SET/CHANGE, SHOW values, HELP/DESCRIBE, etc.

Description: Use the SHOW command to examine the current contents of the ADB, that is, the foreground datasets used for the current analysis. The SHOW command can be used to examine clusters of similar data, the values of individual parameters, or the data contained in entire vectors. Typing SHOW without an option will display a list of the available options.

Examples:

1. The SHOW command can be used to examine the value of a single parameter. For example, the pH of segment 7 of the current ecosystem during September could be inspected by entering:

```
EXAMS > SHOW PH(7,9)
```

Through the use of wild cards (*), the SHOW command can also be used to display the data in an entire vector or row/column of a data matrix. For example, the pH of all segments of the current ecosystem during September could be displayed by entering:

```
EXAMS > SHOW PH(*,9)
```

and the pH of segment 7 through the year could be displayed by:

```
EXAMS > SHOW PH(7,*)
```

S T O R E

Use STORE to download current (ADB) data into the permanent database (UDB).

Related: Control Variables: MCHEM

Commands: CATALOG, ERASE, NAME, RECALL

Syntax: STORE <datatype> [ADB# IN] UDB#

Prompt: Enter ENVIRONMENT, CHEMICAL, LOAD, PRODUCT, HELP or EXIT >

Command parameters:

<datatype> can be CHEMICAL, ENVIRONMENT, LOAD, or PRODUCT (EXAMS uses these four kinds of datasets.)

ADB# IN is an optional explicit specification of MCHEM (see Example 1).

UDB# specifies the accession number or location in the User Database for storage of the current ADB sector (Example 2).

Description: STORE downloads data from activity databases (ADBs) into the permanent User DataBases (UDBs). The data in active use by EXAMS are held in a foreground memory bank (Activity DataBase or ADB) with four sectors, one for each datatype required by EXAMS:

CHEMICAL reactivity and partitioning,

ENVIRONMENTal physico/chemical parameters,

allochthonous chemical LOADings, and

PRODUCT chemistry for generating interconversions among multiple chemicals in an analysis.

When an analysis session is ended (QUIT or EXIT), these data are discarded. Use the STORE command to transfer data from the ADB to the UDB sector of the same datatype for permanent retention of the data.

Examples:

1. Because EXAMS can process several chemicals in a single analysis, the source sector of the chemical activity database should be specified when using the STORE command to download

CHEMICAL data. (This section of the command should be omitted for other data types.) When the ADB# (an integer between 1 and KCHEM) is omitted, the chemical data is taken from the sector of the activity database given by the current value of MCHEM. For example, to STORE data in the UDB, putting ADB sector 1 into the chemical UDB under catalog/accession number 9 and ADB sector 2 into UDB sector 14:

Either:

```
EXAMS > SET MCHEM TO 1

EXAMS > STORE CHEMICAL 9

EXAMS > SET MCHEM TO 2

EXAMS > STORE CHEMICAL 14
```

or, equivalently:

```
EXAMS > STORE CHEMICAL 1 IN 9

EXAMS > STORE CHEMICAL 2 IN 14
```

2. Long-term retention of data required by EXAMS is provided by storage in the "User Database" (UDB, generally resident on a physical device--e.g., a hard disk) for CHEMICALs, ENVIRONMENTs, LOADs, or PRODUCTs. Within each of these UDB sectors, each dataset is CATALOGed via a unique accession number (UDB#). When transferring data between foreground memory (the activity database or ADB) and a UDB, the target location must be specified by the name of the UDB sector and the accession number within the sector. For example, to STORE the current environmental dataset:

```
EXAMS > STORE ENVIR 2

Environment record   2 is in use with
Pond -- AERL code test data
Replace? > NO

Nothing changed.

EXAMS > STORE ENVIR 14

Environment stored:  Phantom Inlet, Bogue Sound Study Data

EXAMS >
```

Note that EXAMS provides a measure of protection against accidental overwriting of existing datasets, an important courtesy in a multi-user environment.

Z E R O

Use the ZERO command to initialize (set to zero) loadings databases or the concentration of pollutant chemicals throughout the ecosystem.

Related: Control variables: MODE
Commands: CONTINUE, RUN

Syntax: ZERO (option)

Options:

PULSE LOADS
LOADS
RESIDUALS

Prompt: The following options are available:

```
PULSE LOADS - zero all pulse loads,
LOADS       - zero all other loads,
RESIDUALS   - zero all pollutant concentrations,
HELP        - this message, or
EXIT        - return to command mode with no action.

ZERO >
```

Description: The ZERO command initializes (sets to zero) the entire suite of allochthonous chemical pulse loadings (IMASS), longer term loadings (stream loads, drift loads, etc.), or the current values of pollutant chemical concentrations throughout the ecosystem. The ZERO command is designed primarily for use during the course of temporally segmented simulation studies. The same effect can be achieved with multiple applications of the CHANGE/SET command; ZERO is a block-mode implementation that reduces the work needed to remove loadings datasets. (See Example 1 in the documentation of the CONTINUE command.)

Examples: 1.

```
EXAMS > SET MODE=2

EXAMS > RECALL CHEMICAL 22

Selected compound is:  Dibromomucktane

EXAMS > RECALL ENVIRON 17

Selected environment is:  Albemarle Sound - Bogue Bank

EXAMS > SET STRL(1,1,13)=.01
```

```
EXAMS > SET IMASS(1)=2.0

EXAMS > SET ISEG(1)=14

EXAMS > SET ICHEM(1)=1

EXAMS > RUN

Simulation beginning for:
Environment: Albemarle Sound - Bogue Bank
Chemical  1: Dibromomucktane

Run complete.

.
.
.

EXAMS > ZERO PULSE LOADS

EXAMS > CONTINUE
```

In this example, an initial-value (MODE=2) analysis is begun by selecting a chemical and an environment, imposing an allochthonous load of chemical 1 on segment 1 under average conditions (i.e., data sector 13, EXAMS' initial default value), and specifying the initial presence (or introduction at time zero) of 2.0 kg of material in segment 14. At the end of the initial RUN segment, one might want to examine the output tables, plot the results, etc. Then, before CONTINUing, the ZERO command is used to remove the pulse load specifications. If this were not done, EXAMS would introduce a second 2.0 kg pulse into segment 14 at the beginning of the continuation segment. Alternatively, the other loadings could have been removed, and the effect of a series of pulse loads could be studied by issuing a sequence of CONTINUE commands.

G L O S S A R Y

ABSER

ABSolute ERror tolerance of integrators.

When the characteristics of the chemical and ecosystem are such as to result in "stiff" equations, numerical errors may lead to small negative numbers in the time series. If desired, the value of ABSER and RELER can be decreased in order to achieve greater precision in the simulation outputs.

ADB

Activity DataBase

FXAMS provides for long-term storage of CHEMical, ENVironmental, transformation PRODuct chemistry, and allochthonous LOADings databases in a User DataBase or UDB. The actual analyses are conducted on particular datasets drawn from these files (or entered via SET/CHANGE). Particular cases are loaded from the UDB into the foreground transient memory of your computer in an Activity DataBase or ADB, using the RECALL command. Because EXAMS simulates the behavior of several (MCHEM) chemicals simultaneously, the ADB for chemicals has MCHEM separate sectors. These data are lost when you EXIT from EXAMS, so be sure to STORE any new or corrected datasets before leaving EXAMS.

ABSOR

ABSORption spectra (wavelength, ion, chemical) Units: /cm/(mole/L)

Mean decadic molar light extinction coefficients in 46 wavelength intervals over 280--825 nm. For wavelength "w" and chemical "c":

ABSOR(w,1,c)	is absorption coefficient of		SH_3	(neutral molecule)
ABSOR(w,2,c)	"	"	"	SH_4^+ (1+ cation)
ABSOR(w,3,c)	"	"	"	SH_5^{2+} (2+ cation)
ABSOR(w,4,c)	"	"	"	SH_6^{3+} (3+ cation)
ABSOR(w,5,c)	"	"	"	SH_2^- (1- anion)
ABSOR(w,6,c)	"	"	"	SH^{2-} (2- anion)
ABSOR(w,7,c)	"	"	"	S^{3-} (3- anion)

ADVPR

ADVection PRoportion (path) Units: n/a Range: > 0 - 1.0

PRoportion of flow ADVected from segment JFRAD that enters ITOAD. The matching (same subscript) members of JFRAD, ITOAD, and ADVPR define an advective hydrologic flow pathway. Although usually 1, ADVPR lets one enter braided channels, etc. The total of ADVPRs for each segment must sum to either 0 or 1, failing which, EXAMS aborts the RUN. The flow data can be inspected by typing SHOW ADV; path numbers are given above each active dataset. Enter data via CHANGE or SET commands.

Additional information available: JFRAD, ITOAD

AEC

Anion Exchange Capacity (segment, month) Units: meq/100 g (dry)

Anion exchange capacity of sediment phase of each segment. Useful in relating sediment sorption (partitioning) of anions to a variable characteristic of system sediments.

AIRTY

AIR mass TYpe (month) Units: letter codes

Select: Rural (default), Urban, Maritime, or Tropospheric

AREA

AREA (segment) Units: m^2

Top plan area of each model segment of the waterbody. For Epilimnion and Littoral segments, AREA is the area of the air-water interface; for Hypolimnion segments AREA is the area of the thermocline; for Benthic segments it is the surface area of the bottom. In the latter case AREA may differ from XSTUR in a dispersive exchange pair because of reduction in exchanging area due to rock outcrops, etc.

ATURB

Atmospheric TURBidity (month) Units: km

Equivalent aerosol layer thickness.

AUDOUT

While the AUDIT directive is in effect, a copy of user inputs and responses is written to the file connected to FORTRAN Logical Unit Number AUDOUT.

BACPL

BACterioPLankton population density (segment, month) Units: cfu/mL

Population density of bacteria capable of degrading xenobiotics.

BNBAC

BeNthic BACteria (segment, month) Units: cfu/100g dry sediment

Population density of benthic bacteria that degrade xenobiotics.

BNMAS

BeNthic bioMASs (segment, month) Units: g(dry)/m^2

Biomass of small benthos--infauna subject to biosorption.

BULKD

BULK Density (segment, month) Units: g/cm^3

Fresh weight per unit volume of benthic sediments.

CEC

Cation Exchange Capacity (segment, month) Units: meq/100g (dry)

Cation exchange capacity of sediment phase in each segment. Useful in relating sediment sorption (partitioning) of cations to a variable characteristic of system sediments.

CHARL

CHARacteristic Length or mixing length (path) Units: m

Average of segment dimensions normal to the exchange interface linking segment numbers JTURB(p) and ITURB(p). The matching (same "p" subscript) members of JTURB, ITURB, CHARL, DSP, and XSTUR together define a dispersive transport pathway. A given segment may have different mixing lengths at different interfaces. CHARL can also be calculated from the distance along a path that connects the centers of segments JTURB(p) and ITURB(p), passing through the interface whose area is XSTUR(p).

See also: DSP, ITURB, JTURB, XSTUR

CHEMNA

CHEMical NAme(s) of compounds (50 characters,chemical) Units: n/a

Do NOT use "CHANGE" or "SFT" to enter names! The NAme for a CHEMical is entered into the database via the command sequence:

EXAMS > CHEMICAL NAME IS nnn...

where "nnn... " can include as many as 50 characters. This name is associated with chemical library entries and is printed in the header information of the appropriate output tables.

CHL

CHLorophylls + pheophytins (segment, month) Units: mg/L

Concentration of chlorophyll plus chlorophyll-like pigments. Used to compute spectral light absorption coefficients due to pigments which absorb light from the water column and thus compete with photolysis of xenobiotics.

CHPAR

CHemical PARent compound (path) Units: n/a Range: 1 - KCHEM

CHPAR(p) gives the ADB location of the parent source of TPROD(p). The matching (same transformation path number "p") members of CHPAR and TPROD give the location numbers in the active database of the parent chemical and the transformation product for pathway "p". For example, "SET CHPAR(p) TO 1", and TPROD(p) to 4, to show that the chemical in ADB sector 4 is produced via transformation of the chemical in ADB sector 1, via process data defined by the remaining members of product chemistry sector "p".

See also: EAYLD, NPROC, RFORM, TPROD, YIELD

CINT

Communications INTerval for dynamic simulations. Units: see TCODE

CINT is the interval between output cycles from the integrators. In Mode 2, CINT can be set to produce any desired output frequency, so long as the resulting reporting interval is $\geq$ 1 hour. When CINT is set to 0.0, EXAMS (Mode 2) sets CINT to report at the 12 equal-increment periods most closely matching the duration specified by (TEND - TINIT). CINT is under full user control only in Mode 2; in Modes 1 and 3 EXAMS itself sets the value of CINT according to the needs of the analysis.

CLOUD

CLOUDiness (month) Units: dimensionless Range: 0 -- 10

Mean monthly cloudiness in tenths of full sky cover.

DEPTH

DEPTH (segment) Units: m

Average vertical depth of each segment.

DFAC

Distribution FACtor (segment, month) Units: dimensionless ratio

Ratio of optical path length to vertical depth, range 1.0-2.0. A vertical light beam has a DFAC of 1.0; a fully diffused light field has a DFAC of 2.0. For whole days, a value of 1.19 is often adequate; EXAMS defaults to this value when the entry for DFAC is outside the range 1.0-2.0.

DISO2

DISsolved O_2 (segment, month) Units: mg/L

Concentration of dissolved oxygen in each segment of ecosystem.

DOC

Dissolved Organic Carbon (segment, month) Units: mg/L

Used for computing spectral light absorption and complexation.

DRFLD

DRiFt LoaD (segment, chemical, month) Units: kg/hour

Drift loadings: aerial drift, direct applications, stack fallout (etc.) of chemical on each system element.

DSP

DiSPersion coefficient (path, month) Units: m^2/hour

Eddy diffusivity to be applied to dispersive exchange pairing "p". The matching (same "p" subscript) members of JTURB, ITURB, CHARL, and XSTUR together define a dispersive transport pathway. In the case of horizontal mixing, DSP is the longitudinal dispersion coefficient; for vertical mixing it may represent exchange across the thermocline or exchanges with bottom sediments. In the latter case DSP is a statistical kinetic composite incorporating direct sorption to the sediment surface, mixing of the sediments by benthos (bioturbation), stirring by demersal fishes, etc.

See also: CHARL, ITURB, JTURB, XSTUR

EAH

Ea for Acid Hydrolysis (form, ion, chemical) Units: kcal/mole

Arrhenius activation energy of specific-acid-catalyzed hydrolysis of chemicals. Matrix indices match those of KAH, giving, for each chemical, data for 3 forms (1: dissolved, 2: solids-sorbed, 3: DOC-complexed) of 7 ionic species (1: neutral; 2, 3, 4: cations; 5, 6, 7: anions). When EAH is non-zero, the second-order rate constant is calculated from:

$$\log K\ (/M/hour) = KAH(f,i,c) - \frac{1000. * EAH(form,ion,chemical)}{4.58 * (TCEL(segment,month) + 273.15)}$$

EAYLD

EA YieLD (path) Units: kcal

EAYLD(p) is activation energy Ea to compute transformation product yield as a function of environmental temperatures (TCEL). When EA YieLD(p) is zero, YIELD(p) gives the dimensionless molar product yield. A non-zero EAYLD(p) invokes a re-evaluation in which YIELD(p) is interpreted as the pre-exponential factor in an Arrhenius-type function, giving product yield as a function of spatially and temporally specific temperatures (TCEL(segment, month)):

$$\log Yield(p) = YIELD(p) - \frac{1000 * EAYLD(path)}{4.58 * (TCEL(segment,month) + 273.15)}$$

See also: CHPAR, NPROC, RFORM, TPROD, YIELD

EBH

Ea for Base Hydrolysis (form, ion, chemical) Units: kcal/mole

Arrhenius activation energy of specific-base catalyzed hydrolysis of chemicals. Matrix indices match those of KBH, giving, for each chemical, data for 3 forms (1: dissolved, 2: solids-sorbed, 3: DOC-complexed) of 7 ionic species (1: neutral, 2, 3, 4: cations, 5, 6, 7: anions). When EBH is non-zero, the second-order rate constant is calculated from:

$$\log K\ (/M/hour) = KBH(f,i,c) - \frac{1000. * EBH(form,ion,chemical)}{4.58 * (TCEL(segment,month) + 273.15)}$$

EHEN

Enthalpy term for HENry's law (chemical) Units: kcal/mole

Used to compute Henry's law constants as a function of TCEL (environmental temperature). When EHEN is non-zero, the Henry's law constant (H) affecting volatilization at a particular (segment, month) is computed from TCEL:

$$\log H = HENRY(chemical) - \frac{1000 * EHEN(chemical)}{4.58\ (TCEL(segment,month) + 273.15)}$$

EK102

Ea K^1O_2 (singlet oxygen) (form, ion, chemical) Units: kcal/mole

Arrhenius activation energy for singlet oxygen photo-oxygenation of chemicals. Matrix indices match those of K102, giving, for each chemical, data for 3 forms (1: dissolved, 2: solids-sorbed, 3: DOC-complexed) of 7 ionic species (1: neutral, 2, 3, 4: cations, 5, 6, 7: anions). When EK102 is non-zero, the second-order rate constant is calculated as:

$$\log K_{(/M/hour)} = K102(f,i,c) - \frac{1000. * EK102\ (form,ion,chemical)}{4.58 * (TCEL(segment,month) + 273.15)}$$

ELEV

ELEVation Units: meters above mean sea level

Ground station elevation.

ENH

Ea for Neutral Hydrolysis (form, ion, chemical) Units: kcal/mole

Arrhenius activation energy for neutral hydrolysis of chemicals. Matrix indices match those of KNH, giving, for each chemical, data for 3 forms (1: dissolved, 2: solids-sorbed, 3: DOC-complexed) of 7 ionic species (1: neutral, 2, 3, 4: cations, 5, 6, 7: anions). When ENH is non-zero, the second-order rate constant is calculated from:

$$\log K_{(/M/hour)} = KNH(f,i,c) - \frac{1000. * ENH\ (form,ion,chemical)}{4.58 * (TCEL(segment,month) + 273.15)}$$

EOX

Ea OXidation (form, ion, chemical) Units: kcal/mole

Arrhenius activation energy for oxidative transformations of chemicals. Matrix indices match those of KOX, giving, for each chemical, data for 3 forms (1: dissolved, 2: solids-sorbed, 3:DOC-complexed) of 7 ionic species (1: neutral, 2, 3, 4: cations, 5, 6, 7: anions). When EOX is non-zero, the second-order rate constant is calculated from:

$$\log K_{(/M/hour)} = KOX(f,i,c) - \frac{1000. * EOX\ (form,ion,chemical)}{4.58 * (TCEL(segment,month) + 273.15)}$$

EPK

Enthalpy term for pK (ion, chemical) Units: kcal/mole

When EPK is non-zero, pK is computed as a function of temperature via:

$$\log pK = PK(i,c) - \frac{1000. * EPK(ion,chemical)}{4.58 * (TCEL(segment,month) + 273.15)}$$

The vector indices for EPK ("c" the chemical) are:

EPK(1,c) contains datum for generation of SH_4^+ from SH_3

EPK(2,c) contains datum for generation of SH_5^{2+} from SH_4^+

EPK(3,c) " " " " " SH_6^{3+} " SH_5^{2+}

EPK(4,c) " " " " " SH_2^- " SH_3

EPK(5,c) " " " " " SH^{2-} " SH^-

EPK(6,c) " " " " " S^{3-} " SH^{2-}

ERED

Ea REDuction (form, ion, chemical) Units: kcal/mole

Arrhenius activation energy for reductive transformations of chemicals. Matrix indices match those of KRED, giving, for each chemical, data for 3 forms (1: dissolved, 2: solids-sorbed, 3: DOC-complexed) of 7 ionic species (1: neutral, 2, 3, 4: cations, 5, 6, 7: anions). When ERED is non-zero, the second-order rate constant is calculated as:

$$\log K\ (/M/hour) = KRED(f,i,c) - \frac{1000. * FRED\ (form,ion,chemical)}{4.58 * (TCEL(segment,month) + 273.15)}$$

ESOL

Enthalpy term for SOLubility (ion, chemical) Units: kcal/mole

ESOL describes chemical solubility as a function of temperature (TCEL). The matrix indices ("c" the chemical) denote:

ESOL(1,c) -- datum for solubility of SH_3 (neutral molecule)

ESOL(2,c) -- " " " " SH_4^+ (1+ cation)

ESOL(3,c) -- " " " " SH_5^{2-} (2+ cation)

ESOL(4,c) -- " " " " SH_6^{3+} (3+ cation)

ESOL(5,c) -- " " " " SH^- (1- anion)

ESOL(6,c) -- " " " " SH^{2-} (2- anion)

ESOL(7,c) -- " " " " S^{3-} (3- anion)

EVAP

EVAPoration (seqment, month) Units: mm/month

(Monthly) evaporative water losses from ecosystem seqments.

EVPR

Molar hEat of VaPoRization (chemical) Units: kcal/mole

Enthalpy term for computing vapor pressure as a function of TCEL (environmental temperature (segment,month)). When EVPR is non-zero, vapor pressure V_a is computed from:

$$\log V_a = \text{VAPR(chemical)} - \frac{1000 * \text{EVPR(chemical)}}{4.58\ (\text{TCEL(segment,month)} + 273.15)}$$

FIXFIL

FIXFIL signals the existence of output data for LISTs and PLOTs.

To access results from a prior run, "SET FIXFIL to 1." FIXFIL is set to zero when FXAMS is invoked, so that the LIST and PLOT commands are protected from attempts to access non-existent output data files. When results exist from a previous simulation, you can reset FIXFIL to 1 in order to gain access to them.

FROC

FRaction Organic Carbon (segment, month) Units: dimensionless

Organic carbon content of solids as fraction of dry weight. FROC is coupled to KOC to generate the sediment partition coefficient for neutral chemicals (SH3) as a function of a property (organic carbon content) of the sediment.

HENRY

HENRY's law constant (chemical) Units: atmosphere-m^3/mole

Used in computation of air/water exchange rates (volatilization). If parameter EHEN is non-zero, HENRY is used as the pre-exponential factor in computing the Henry's law constant H as a function of environmental temperatures (TCEL):

$$\log H = \text{HENRY(chemical)} - \frac{1000 * \text{EHEN(chemical)}}{4.58\ (\text{TCEL(segment,month)} + 273.15)}$$

ICHEM

I CHEMical (event) Units: n/a Range: 1 -- KCHEM

Event "e" is a pulse of chemical number ICHEM(e) in the active database ICHEM identifies the location in the Activity Database (ADB) of the chemical entering the ecosystem via pulse load event "e". When, for example, chemical data are loaded into ADB sector 3 (whether RECALLed from the User Database Library (UDL) (via, for example, the command sequence "RECALL CHEM 7 AS 3") or entered as new data), ICHEM(e) can be SET to 3 to create a pulse load event of that chemical.

See also: IDAY, IMASS, IMON, ISEG.

IDAY

I DAY (event) Units: n/a Range: 1 -- 31

Pulse load event "e" takes place on day IDAY(e) of month IMON(e). The pulse load data are organized by vertical event columns, that is, the set of pulse load variables (IMASS(e), ICHEM(e), ISEG(e), IMON(e), and IDAY(e)) with the same vector subscript describes a single chemical pulse event. Thus a pulse of chemical ICHEM(e), of magnitude IMASS(e), is released into segment ISEG(e) on day IDAY(e) of month IMON(e). During mode 2 simulations, IDAY and IMON are inoperative.

See also: ICHEM, IMASS, IMON, ISEG.

IMASS

Initial MASS (event) Units: kg

IMASS gives the magnitude of chemical pulse load event "e". In mode 2, pulses are entered at time 0 (i.e., as initial conditions), and at the outset of each CONTINUation of the simulation. In mode 3, IMON and IDAY specify the date of the load events. An event recurs in each year of the RUN or CONTINUed simulation. The pulse load data are organized by vertical event columns, that is, the series of pulse load variables (IMASS, ICHEM, ISEG, IMON, and IDAY) with the same vector subscript describes a single event.

See also: ICHEM, IDAY, IMON, ISEG.

IMON

I MONth (event) Units: n/a Range: 1--12

Pulse load event "e" takes place on day IDAY(e) of month IMON(e). The pulse load data are organized by vertical event columns, that is, the set of pulse load variables (IMASS(e), ICHEM(e), ISEG(e), IMON(e), and IDAY(e)) with the same vector subscript describes a single chemical pulse event. Thus a pulse of chemical ICHEM(e), of magnitude IMASS(e),

is released into segment ISEG(e) on day IDAY(e) of month IMON(e). During mode 2 simulations, IDAY and IMON are inoperative.

See also: IDAY, ICHEM, IMASS, ISEG.

ISEG

I SEGment (event) Units: n/a Range: 1--KOUNT

Pulse load event "e" loads chemical ICHEM(e) on segment ISEG(e). Any segment can receive a pulse load. Should the pulse loads increase the FREE concentration of unionized chemical above 10-5 M (or half its aqueous solubility, whichever is less), the size of the event is reduced, to avoid violating the linearizing assumptions used to create EXAMS. The pulse load data are organized by vertical event columns, that is, the pulse load variables having the same vector subscript define a single chemical pulse event.

See also: ICHEM, IDAY, IMASS, IMON.

ITOAD

I TO ADvection (path) Units: n/a Range: 0--KOUNT (0 = export)

Chemicals are advected to segment ITOAD(p) from segment JFRAD(p). The matching (same subscript) members of JFRAD, ITOAD, and ADVPR define an advective hydrologic flow pathway carrying entrained chemicals and solids through the waterbody. When ITOAD(p) is 0, the pathway advects water and entrained substances across system boundaries, i.e., ITOAD(p) = 0 specifies an export pathway. The flow data can be inspected by typing "SHOW ADV"; path numbers are given above each active dataset. Enter data with SET or CHANGE commands.

See also: JFRAD, ADVPR

ITURB

I TURbulent dispersion (path) Units: n/a Range: 0--KOUNT

Segments ITURB(p) and JTURB(p) exchange via turbulent dispersion. The matching (same "p" subscript) members of ITURB, JTURB, CHARL, DSP, and XSTUR together define a dispersive transport pathway; ITURB(p) and JTURB(p) indicate which segments are linked by dispersive transport pathway "p". A "0" in ITURB paired with a non-zero segment number in JTURB denotes a boundary condition with a pure (zero chemical) waterbody. The input data can be examined via SHOW TURBULENCE; pathway numbers are shown with each dataset.

See also: CHARL, DSP, JTURB, XSTUR.

IUNIT

IUNIT controls the printing of diagnostics from the integrators.

Normally zero (off), it may be turned on when problems occur. To manually set IUNIT to generate integrator diagnostic messages, SET IUNIT TO 1. The message generator can be disabled at any time by SETting IUNIT to 0.

JFRAD

J FRom ADvection (path) Units: n/a Range: 1--KOUNT

Chemicals are advected from segment JFRAD(p) to segment ITOAD(p). The matching (same subscript) members of JFRAD, ITOAD, and ADVPR define an advective hydrologic flow pathway. EXAMS computes the total net flow available for advection from segment JFRAD(p). Of the total flow, the fraction ADVPR(p) flows from segment JFRAD(p) into segment ITOAD(p). The hydrologic flow carries an entrained mass of chemical along the pathway. The flow specifications can be inspected by typing SHOW ADV; pathway numbers are given above each active dataset. Enter data with SET or CHANGE commands.

See also: ITOAD, ADVPR

JTURB

J TURBulent dispersion (path) Units: n/a Range: 0--KOUNT

Segments JTURB(p) and ITURB(p) exchange via turbulent dispersion. The matching (same "p" subscript) members of JTURB, ITURB, CHARL, DSP, and XSTUR together define a dispersive transport pathway; JTURB(p) and ITURB(p) indicate which segments are linked by dispersive transport pathway "p". A "0" in JTURB paired with a non-zero segment number in ITURB denotes a boundary condition with a pure (zero chemical) water-body. The input data can be examined via SHOW TURBULENCF; pathway numbers are shown with each dataset.

See also: CHARL, DSP, ITURB, XSTUR

KAH

KAcid Hydrolysis (form, ion, chemical) Units: per mole $[H^+]$/hour

Second-order rate constant for specific-acid-catalyzed hydrolysis of chemicals. When the matching (same subscripts) Arrhenius activation energy (EAH) is zero, KAH is interpreted as the second-order rate constant. When the matching entry in EAH is non-zero, KAH is interpreted as the (Briggsian) logarithm of the frequency factor in an Arrhenius equation, and the 2nd-order rate constant is computed as a function of segment temperatures TCEL. Matrix indices refer to 3 forms -- 1: aqueous, 2: solids-sorbed, and 3: DOC-complexed; by 7 ions-- 1: neutral, 2-4: cations, and 5-7: anions.

KBACS

KBACteria benthoS (form, ion, chemical) Units: /(cfu/mL)/hr

Second-order rate constants -- benthic sediment bacterial biolysis of chemicals. When the matching (same subscripts) Q-10 (QTBAS) is zero, KBACS is interpreted as the second-order rate constant. When the matching entry in QTBAS is non-zero, KBACS is interpreted as the numerical value of the second-order rate constant at 20° C, and local values of the rate constant are computed as a function of temperature (TCEL) in each ecosystem segment. Indices refer to 4 forms -- 1: aqueous, 2: solids-sorbed, 3: DOC-complexed, and 4:bio-sorbed; by 7 ions-- 1: neutral, 2-4: cations, and 5-7: anions.

KBACW

KBACterioplankton Water (form, ion, chemical) Units: /(cfu/mL)/hr

Second-order rate constants K for water column bacterial biolysis of chemicals. When the matching (same subscripts) Q-10 (QTBAW) is zero, KBACW is interpreted as the second-order rate constant. When the matching entry in QTBAW is non-zero, KBACW is interpreted as the numerical value of the second-order rate constant at 20° C, and local values of the rate constant are computed as a function of temperature (TCEL) in each ecosystem segment. Indices refer to 4 forms -- 1: aqueous, 2: solids-sorbed, 3: DOC-complexed, and 4:bio-sorbed; by 7 ions-- 1: neutral, 2-4: cations, and 5-7: anions.

KBH

KBase Hydrolysis (form, ion, chemical) Units: per mole [OH^-]/hour

Second-order rate constant for specific-base-catalyzed hydrolysis of chemicals. When the matching (same subscripts) Arrhenius activation energy (EBH) is zero, KBH is interpreted as the second-order rate constant. When the matching entry in EBH is non-zero, KBH is interpreted as the (Briggsian) logarithm of the frequency factor in an Arrhenius equation, and the 2nd-order rate constant is computed as a function of segment temperatures TCEL. Matrix indices refer to 3 forms -- 1: aqueous, 2: solids-sorbed, and 3: DOC-complexed; by 7 ions -- 1: neutral, 2-4: cations, and 5-7: anions.

KCHEM

Number of chemicals under review in current study. Units: n/a

KDP

KDirect Photolysis (ion, chemical) Units: reciprocal hours

Estimated photolysis rates--use only when ABSOR is unavailable. KDP is an annual average for cloudless conditions at RFLAT, where

KDP(1,c) refer to photolysis of neutral molecules SH_3

KDP(2,c) " " " " singly charged cations SH_4^+

KDP(3,c) " " " " doubly charged cations SH_5^{2+}

KDP(4,c) " " " " triply charged cations SH_6^{3+}

KDP(5,c) " " " " singly charged anions SH^-

KDP(6,c) " " " " doubly charged anions SH^{2-}

KDP(7,c) " " " " triply charged anions S^{3-}

KIEC

Kp for Ion Exchange Capacity (ion, chemical) Units: Kp /(meq/100g dry)

Coefficient relating Kp of ions to exchange capacity of sediments. KIEC times CEC(seg, month) (or AEC) gives Kp for sorption of ions with solid phases. Overridden by explicit (non-zero) values of KPS.

KIEC(1,c) contains datum for relating sorption of SH_4^+ to C.E.C.

KIEC(2,c) " " " " " " SH_5^{2+} "

KIEC(3,c) " " " " " " SH_6^{3+} "

KIEC(4,c) " " " " " " SH_2^- to A.E.C.

KIEC(5,c) " " " " " " SH_{2-} "

KIEC(6,c) " " " " " " S_{3-} "

KINOUT

Logical Unit Number for writing results of numerical integration to kinetics plotting file.

KNH

KNeutral Hydrolysis (form, ion, chemical) Units: per hour

Pseudo-first-order rate constants for neutral hydrolysis of chemicals. When the matching (same subscripts) Arrhenius activation energy (ENH) is zero, KNH is interpreted as the second-order rate constant. When the matching entry in EN is non-zero, KNH is interpreted as the (Briggsian) logarithm of the frequency factor in an Arrhenius equation, and the 2nd-order rate constant is computed as a function of segment temperatures TCEL. Matrix indices refer to 3 forms -- 1: aqueous, 2: solids-sorbed, and 3: DOC-complexed; by 7 ions -- 1: neutral, 2-4: cations, and 5-7: anions.

KOC

Koc(chemical) Units: ((mg/kg)/(mg/L)) / (organic carbon fraction)

KOC is partition coefficient (Kp) keyed to organic carbon content FROC(s, m) of the sediment solids in each (s) segment, during each (m) month of simulation of chemical behavior in the system. Multiplication of KOC by the organic carbon fraction FROC(s) of the solids in each segment yields the partition coefficient (Kp) for sorption of unionized (SH_3) species with those solids:

Kp(chemical, segment, month) = KOC(chemical) * FROC(segment, month)

KOUNT

Number of segments used to define current ecosystem. Units: n/a

KOW

Octanol-Water partition coefficent (chemical) Units: (mg/L)/(mg/L)

Kow is an experimentally determined chemical descriptor. Kow (KOW(c)) can be used to estimate Koc (c.f.), and thus relate the Kp of a chemical to the organic carbon content of sediments.

KOX

K OXidation (form, ion, chemical) Units: per mole [OXRAD] /hour

Second-order rate constants for free-radical (OXRAD) oxidation of chemicals. When the matching (same subscripts) Arrhenius activation energy (EOX) is zero, KOX is interpreted as the second-order rate constant. When the matching entry in EOX is non-zero, KOX is interpreted as the (Briggsian) logarithm of the frequency factor in an Arrhenius equation, and the 2nd-order rate constant is computed as a function of segment temperatures TCEL. Matrix indices refer to 3 forms -- 1: aqueous, 2: solids-sorbed, and 3: DOC-complexed; by 7 ions -- 1: neutral, 2-4: cations, and 5-7: anions.

KO2

KO_2(segment, month) Units: cm/hour

Oxygen exchange constant or piston velocity at 20° C in each ecosystem segment.

KPB

KP for Biomass (ion, chemical) Units: (ug/g) / (mg/L)

Partition coefficient (Kp) for computing equilibrium biosorption. The "ion" subscripts ("c" is the chemical) identify:

KPB(1,c) -- datum for biosorption of SH_3 (neutral molecule)

KPB(2,c) -- datum for biosorption of SH_4^+ (1+ cation)

KPB(3,c) -- " " " " SH_5^{2+} (2+ cation)

KPB(4,c) -- " " " " SH_6^{3+} (3+ cation)

KPB(5,c) -- " " " " SH^- (1- anion)

KPB(6,c) -- " " " " SH^{2-} (2- anion)

KPB(7,c) -- " " " " S^{3-} (3- anion)

KPDOC

KPDissolved Organic Carbon (ion, chemical) Units: (ug/g)/(mg/L)

Partition coefficient (Kp) for equilibrium complexation with DOC. The "ion" subscripts ("c" is the chemical) identify:

KPDOC(1,c) -- datum for complexation of SH_3 (neutral molecule)

KPDOC(2,c) -- datum for complexation of SH_4^+ (1+ cation)

KPDOC(3,c) -- " " " " SH_5^{2+} (2+ cation)

KPDOC(4,c) -- " " " " SH_6^{3+} (3+ cation)

KPDOC(5,c) -- " " " " SH^- (1- anion)

KPDOC(6,c) -- " " " " SH^{2-} (2- anion)

KPDOC(7,c) -- " " " " S^{3-} (3- anion)

KPS

KP for Sediment solids (ion, chemical) Units: (mg/kg)/(mg/L)

Partition coefficients (Kp) for computing sorption with sediments. The "ion" subscripts ("c" is the chemical) identify:

KPS(1,c) -- datum for sorption of SH_3 (neutral molecule)

KPS(2,c) -- datum for sorption of SH_4^+ (1+ cation)

KPS(3,c) -- " " " " SH_5^{2+} (2+ cation)

KPS(4,c) -- " " " " SH_6^{3+} (3+ cation)

KPS(5,c) -- " " " " SH^- (1- anion)

KPS(6,c) -- " " " " SH^{2-} (2- anion)

KPS(7,c) -- " " " " S^{3-} (3- anion)

KRED

KREDuction (form, ion, chemical) Units: per mole [REDAG] /hour

Second-order rate constants for REDucing AGent chemical reduction of compounds. When the matching (same subscripts) Arrhenius activation energy (ERED) is zero, KRED is interpreted as the second-order rate constant. When the matching entry in ERED is non-zero, KRED is interpreted as the (Briggsian) logarithm of the frequency factor in an Arrhenius equation, and the 2nd-order rate constant is computed as a function of segment temperatures TCEL. Matrix indices refer to 3 forms -- 1: aqueous, 2: solids-sorbed, and 3: DOC-complexed; by 7 ions -- 1: neutral, 2-4: cations, and 5-7: anions.

KVO

KVOlatilization (chemical) Units: dimensionless ratio

Liquid-phase transport resistance, as ratio to reaeration rate.

K1O2

K1O2(singlet oxygen) (form, ion, chemical) Units: per M [$^1O_2$] /hr

Second-order rate constants for singlet oxygen photo-oxygenation of chemicals. When the matching (same subscripts) Arrhenius activation energy (EK1O2) is zero, K1O2 is interpreted as the second-order rate constant. When the matching entry in EK1O2 is non-zero, K1O2 is interpreted as the (Briggsian) logarithm of the frequency factor in an Arrhenius equation, and the 2nd-order rate constant is computed as a function of segment temperatures TCEL. Matrix indices refer to 3 forms -- 1: aqueous, 2: solids-sorbed, and 3: DOC-complexed; by 7 ions -- 1: neutral, 2-4: cations, and 5-7: anions.

LAMAX

LAMbda MAXimum (ion, chemical) Units: nanometers

Wavelength of maximum absorption of light by each ionic species, or wavelength of maximum overlap of solar spectrum and chemical's absorption spectrum (of each ion). Indices match with KDP matrix. LAMAX selects the wavelengths used to compute light extinction factors for photochemical transformation, in those cases where the absorption spectrum of the compound is not available, but the results of simple photochemical experiments can be used as a coarse estimate of rates of photochemical transformations (i.e., KDP > 0.0). When set to zero, LAMAX defaults to 300 nm.

LAT

LATitude Units: degrees and tenths (e.g., 37.24)

Geographic latitude of the ecosystem.

LENG

LENGth (segment) Units: m

Length of a reach -- used to compute volume, area, depth.

LOADNM

LOADings database NaMe (50 characters) Units: n/a

Do NOT use "CHANGE" or "SET" to enter names! The NaMe for a LOADings database is entered via the command sequence:

EXAMS > LOAD NAME IS nnn...

where "nnn... " can include as many as 50 characters. This name is associated with chemical loadings database library entries, so that load patterns can be found in the catalog. The Ith character can be corrected with a CHANGE or SET command. For example, to repair the 7th character, "SET LOADNM(7) TO ... ."

LONG

LONGitude Units: degrees and tenths (e.g., 154.2)

Geographic longitude of the ecosystem.

MCHEM

M CHEMical Units: n/a

Number of chemical in activity data base.

MODE

MODE sets the operating "mode" of EXAMS.

Three operating modes are available; these are selected by SETting MODE to 1, 2, or 3.

MODE	Operational characteristics of EXAMS
1	Long-term (steady-state) analysis.
2	Pulse analysis -- specifiable initial chemical mass (IMASS) and time frame, time-invariant environment.
3	Monthly environmental data, daily pulse loads IMASS and monthly chemical loadings of other types.

MONTH

MONTH Units: n/a

Set MONTH to inspect a specific block of environmental data.

MWT

Gram Molecular WeighT (chemical) Units: g/mole

Molecular weight of the neutral species of each study chemical. Changes in molecular weight due to ionization are neglected.

NPROC

Number of PROCess (path) Units: n/a Range: 1--9

Signals the type of process transforming CHPAR(p) into TPROD(p).

NPROC can be set to the following:

1 --> specific acid hydrolysis
2 --> neutral hydrolysis
3 --> specific base hydrolysis
4 --> direct photolysis
5 --> singlet oxygen reactions
6 --> free radical oxidation
7 --> water column bacterial biolysis
8 --> benthic sediment bacterial biolysis
9 --> reductions, e.g., reductive dechlorination

See also: CHPAR, EAYLD, RFORM, TPROD, YIELD

NPSED

Non-Point-Source SEDiment (segment, month) Units: kg/hour

Non-point-source sediment loads entering ecosystem segments.

NPSFL

Non-Point-Source FLow (segment, month) Units: m^3/hour

Non-point-source water flow entering ecosystem segments.

NPSLD

Non-Point-Source LoaD (segment, chemical, month) Units: kg/hour

Chemical loadings entering segments via non-point sources.

NYEAR

Number of YEARs Units: n/a

NYEAR is number of years to be simulated for a mode 3 run.

OXRAD

OXidant RADicals (month) Units: moles/L

Concentration of environmental oxidants in near-surface waters (e.g., peroxy radicals). EXAMS computes segment-specific oxidant concentrations using ultra-violet light extinction in the system.

OZONE

OZONE (month) Units: centimeters NTP Typically 0.2 -- 0.3 cm

Mean (monthly) ozone (O_3) content of atmosphere.

PCPLD

PreCiPitation LoaD (segment, chemical, month) Units: kg/hour

Chemical loadings entering each segment via rainfall.

PCTWA

PerCenT WAter (segment, month) Units: dimensionless

Percent water in bottom sediments of benthic segments. Elements of these vectors that correspond to water column segments are not used (dummy values). PCTWA should be expressed as the conventional soil-science variable (the fresh weight : dry weight ratio times 100); all values must be greater than or equal to 100. An entry in PCTWA that is less than 100.0 for a benthic segment raises an error condition, and control is returned to the user for correction of the input data.

PH

pH (segment, month) Units: pH units

The negative value of the power to which 10 is raised in order to obtain the temporally averaged concentration of hydronium ions [H3O+] in gram-equivalents per liter.

PK

pK (ion, chemical)

Negative of base-10 logarithm of acid/base dissociation constants. When the matching value in the EPK matrix is zero, PK(i, c) is taken as the pK value. (To "match" is to have the same subscript values.) When EPK(i, c) is non-zero, PK is taken as the base-10 logarithm of the pre-exponential factor in the equation for pK as a function of environmental temperature TCEL, that is,

$$\log pK = PK(i,c) - \frac{1000\ EPK(ion,chemical)}{4.58\ (TCEL(segment,month) + 273.15)}$$

The vector indices for PK ("c" the chemical) are:

PK(1,c) contains datum for generation of SH_4^+ from SH_3

PK(2,c) " " " " " SH_5^{2+} from SH_4^+

PK(3,c) " " " " " SH_6^{3+} " SH_5^{2+}

PK(4,c) " " " " " SH_2^- " SH_3

PK(5,c) " " " " " SH^{2-} " SH^-

PK(6,c) " " " " " S^{3-} " SH^{2-}

PLMAS

PLanktonic bioMASs (segment, month) Units: mg (dry weight)/L

Total plankton subject to biosorption of xenobiotic chemicals.

POH

pOH (segment, month) Units: pOH units

The negative value of the power to which 10 is raised in order to obtain the temporally averaged concentration of hydroxide [OH-] ions in gram-equivalents per liter.

PRINTR

Logical Unit Number used for printing results on a line printer.

PRODNM

PRODuct chemistry database NaMe (50 characters) Units: n/a

Do NOT use "CHANGE" or "SET" to enter names! The NaMe for a PRODuct chemistry database is entered via the command sequence:

EXAMS > PRODUCT NAME IS nnn...

where "nnn... " can include as many as 50 characters. This name is associated with product chemistry database library entries, so that databases can be found in the catalog. Use a CHANGE or SET command to repair single characters in the name. For example, to repair character seven, enter "SET PRODNM(7) TO ... ."

PRSW

PRint SWitch Units: n/a

PRSW is a switch for controlling printing options. In mode 3, when PRSW is set to 0 (the default), average values of the environmental

parameters are recorded in the run log. When PRSW is 1, a separate table is produced for each (monthly) data set, except for those values which are invariant (VOL etc.).

QTBAS

Q Ten BActeria benthoS (form, ion, chemical) Units: dimensionless

Q-10 values for benthic bacterial biolysis (see KBACS) of chemical. "Q-10" is the increase in the second-order rate constant due to a 10° C increase in temperature. Indices refer to 28 molecular spp: 4 forms -- 1: aqueous, 2: solids-sorbed, 3: DOC-complexed, and 4: bio-sorbed; by 7 ions -- 1: neutral, 2-4: cations, and 5-7: anions. When QTBAS is non-zero, the matching (same subscripts) rate constant is computed as:

$$Kbacs(f,i,c) = QTBAS(f,i,c)^{(TCEL(seg,month)-20)/10} * KBACS(f,i,c)$$

QTBAW

Q Ten BActeria Water (form, ion, chemical) Units: dimensionless

Q-10 values for bacterioplankton biolysis (see KBACW) of chemical. "Q-10" is the increase in the second-order rate constant due to a 10° C increase in temperature. Indices refer to 28 molecular spp: 4 forms -- 1: aqueous, 2: solids-sorbed, 3: DOC-complexed, and 4: bio-sorbed; by 7 ions -- 1: neutral, 2-4: cations, and 5-7: anions. When QTBAW is non-zero, the matching (same subscripts) rate constant is computed as:

$$Kbacw(f,i,c) = QTBAW(f,i,c)^{(TCEL(seg,month)-20)/10} * KBACW(f,i,c)$$

QUANT

QUANTum yield (form, ion, chemical) Units: dimensionless

Reaction quantum yield for direct photolysis of chemicals -- fraction of the total light quanta absorbed by a chemical that results in transformations. Separate values (21) for each potential molecular type of each chemical allow the effects of speciation and sorption on reactivity to be specified in detail. The matrix of 21 values specifies quantum yields for the (3) physical forms: (1) dissolved, (2) sediment-sorbed, and (3) DOC-complexed; of each of (7) possible chemical species: neutral molecules (1), cations (2-4), and anions (5-7). (QUANT is an efficiency.)

RAIN

RAINfall (month) Units: mm/month

Average (monthly) rainfall in geographic area of system.

RANUNT

Logical Unit Number for the UTILITY file support.

The UTILITY file is used for retrieving and storing chemical and environmental parameters, for supporting the on-line assistance facility, and to support the SYSTEM PARAMETERS operations.

REDAG

REDucing AGents (segment, month) Units: moles/L

Molar concentration of reducing agents in each system segment.

RELER

RELative ERror tolerance for integrators.

When the characteristics of the chemical and ecosystem are such as to result in "stiff" equations, numerical errors may lead to small negative numbers in the time series. If desired, the value of ABSER and RELER can be decreased in order to achieve greater precision in the simulation outputs.

RFLAT

ReFerence LATitude (ion, chemical) Units: degrees (e.g., 40.72)

(RFLAT - LAT) corrects for N/S displacement of the ecosystem LAT from the location (RFLAT) of a matched (same subscript) KDP.

RFLAT(1,c) refer to photolysis of neutral molecules SH_3

RFLAT(2,c) " " " " singly charged cations SH_4^+

RFLAT(3,c) " " " " doubly charged cations SH_5^{2+}

RFLAT(4,c) " " " " triply charged cations SH_6^{3+}

RFLAT(5,c) " " " " singly charged anions SH^-

RFLAT(6,c) " " " " doubly charged anions SH^{2-}

RFLAT(7,c) " " " " triply charged anions S^{3-}

RFORM

Reactive FORM (path) Units: n/a Range: 1--32

RFORM gives the reactive molecular form (ionic species in each of the possible sorptive states) of CHPAR(p) resulting in product TPROD(p). The table shows the value of RFORM for each molecular entity, including values for total dissolved (29), solids-sorbed (30), etc.

Ionic spp.	Neutral	Cations			Anions			Total
& valence :	(0)	(1+)	(2+)	(3+)	(1-)	(2-)	(3-)	(all)
Forms:								
Dissolved	1	5	9	13	17	21	25	29
Solids-sorbed	2	6	10	14	18	22	26	30
DOC-complexed	3	7	11	15	19	23	27	31
Biosorbed	4	8	12	16	20	24	28	32

See also: CHPAR, EAYLD, NPROC, TPROD, YIELD

RHUM

Relative HUMidity (month) Units: %, i.e., saturation = 100% R.H.

Mean (monthly) relative humidity during daylight hours. Data typical of daylight hours are needed because their primary use is to characterize light transmission in the atmosphere.

RPTOUT

Logical Unit Number for data written to tabular report file.

SEELD

SEEpage LoaD (segment, chemical, month) Units: kg/hour

Chemical loadings entering the system via "interflows" or seepage (all sub-surface water flows entering the system, (usually) via a benthic segment).

SEEPS

SEEPage flowS (segment, month) Units: m^3/hour

Interflow (subsurface water flow, seepage) entering each segment. SEEPS usually enter via a benthic segment. SEEPS are assumed to lack an entrained sediment flow, that is, they are flows of water only.

SOL

SOLubility (ion, chemical) Units: mg/L

Aqueous solubility of each species (neutral molecule + all ions). When the matching value in the ESOL matrix is zero, SOL(i, c) is taken as the aqueous solubility in mg/L. (To "match" is to have the same subscript values.) When ESOL(i, c) is non-zero, SOL(i, c) is taken as the base-10 logarithm of the pre-exponential factor of the equation describing the MOLAR solubility of the species as a function of environmental temperature (TCEL). The vector indices for SOL are given in the text describing ESOL. Solubility must be specified, because it is used as a constraint on loads.

SPARE2

SPFLG

SPecies FLaGs (ion, chemical) -- can be "1" (exists) or "0".

This vector of "flags" or "switches" shows which ions exist. Set the flags ("SET SPFLG(i, c) TO 1") when entering chemical data in order to show EXAMS the ionic structure of the chemical.

SPFLG(1) set (=1) signals that the neutral molecule SH_3 exists.

SPFLG(2) set signals existence of singly charged cation SH_4^+

SPFLG(3) " " " " doubly " " SH_5^{2+}

SPFLG(4) " " " " triply " " SH_6^{3+}

SPFLG(5) " " " " singly " anion SH_2^-

SPFLG(6) " " " " doubly " " SH^{2-}

SPFLG(7) " " " " triply " " S^{3-}

SSOUT

Logical Unit Number for data written to plotting file containing EXAMS' steady-state chemical concentrations.

STFLO

STream FLOws (segment, month) Units: m^3/hour

Flow into head reach of river or estuary; segment tributaries and creeks or other streamflows entering a lake or pond. Note that STFLO represents stream flow entering system segments from external sources ONLY. EXAMS itself computes hydrologic flows among segments that are part of the waterbody being studied, via the specified advective and dispersive flow patterns (see JFRAD, JTURB, etc.) Therefore, do NOT compute net water balances for each segment and enter these into the database--enter ONLY those flows entering the system across external boundaries!

STRLD

STReam LoaD (segment, chemical, month) Units: kg/hour

Chemical loadings entering ecosystem segments via stream flow.

STSED

STream-borne SEDiment (segment, month) Units: kg/hour

Stream-borne sediment load entering ecosystem segments.

SUSED

SUSpended SEDiment (segment, month) Units: mg/L

Suspended particulate matter -- applicable to the water column only.

SYSTYP

Name of aquatic ecoSYStem TYPe (50 characters) Units: n/a

Do NOT use "CHANGE" or "SET" to enter names! The name of a waterbody is entered into the database via the command sequence:

EXAMS > ENVIRONMENT NAME IS nnn...

where "nnn... " can include as many as 50 characters. This name is associated with environmental library entries (the UDB catalog) and is printed in the header information of the appropriate output tables. Use SET and CHANGE to correct single characters in the name. For example, to correct the seventh character in a name, "CHAN SYSTYP(7) TO ... ."

TCEL

Temperature CELcius (segment, month) Units: degrees C

Average temperature of ecosystem segments. Used (as enabled by input data) to compute effects of temperature on transformation rates and other properties of chemicals.

TCODE

The value of Time CODE sets the units of TINIT, TEND, and CINT.

TCODE can be SET to 1 (hours), 2 (days), 3 (months), or 4 (years). TCODE is under full user control only in Mode 2. In mode 2, TCODE controls the time frame of the study. For example, given TINIT=0., TEND=24., and CINT=2.; CHANging TCODE from 1 to 3 converts a 0-24 hour study into 0-24 months, with bimonthly reports. In mode 1, EXAMS selects the units for reporting results, from the probable half-life of the study chemical(s). In mode 3, a RUN encompasses one year or longer, and the timing is set to produce standard outputs.

TEND

Time END for a dynamic simulation segment. Units: see TCODE

A simulation segment encompasses the period TINIT through TEND. At the end of each integration, TINIT is reset to TEND. The simulation can be extended by invoking the "CONTINUE" command; EXAMS will then request a new value of TEND. Pulse loads (IMASS) and longer-term chemical loads (STRLD, NPSLD, etc.) can be modified or deleted during the pause between simulation segments.

TINIT

Time INITial for a dynamic simulation segment. Units: see TCODE

A simulation RUN encompasses the period TINIT through TEND. At the end of each integration, TEND is transferred to TINIT. The simulation results can be evaluated, and the study continued via the "CONTINUE" command. EXAMS will note the new value of TINIT and request a new endpoint. Pulse and other chemical loadings can be modified or deleted between simulation segments.

TPROD

Transformation PRODuct (path) Units:n/a Range: 1-KCHEM

TPROD(p) -- ADB location of the transformation product of CHPAR(p). The matching (same transformation path number "p") members of CHPAR and TPROD give the location numbers in the active database of the parent chemical and the transformation product for pathway "p". For example, SET CHPAR(p) TO 1, and TPROD(p) to 4, to show that the chemical in ADB sector 4 is produced via transformation of the chemical in ADB sector 1, via process data defined by the remaining members of product chemistry sector "p".

See also: CHPAR, EAYLD, NPROC, RFORM, YIELD

TTYIN

Logical Unit Number for interactive input commands.

TTYOUT

Logical Unit Number for output error messages and warnings, and for EXAMS' interactive responses.

TYPE

Segment TYPE (segment) Units: letter codes

Letter codes designating segment types used to define ecosystems. Available types: Littoral, Epilimnion, Hypolimnion, and Benthic.

UDB

User DataBase

Long-term retention of data required by EXAMS is provided by storage in the "User Database" (UDB, generally resident on a physical device, e.g., a hard disk) for CHEMICALs, ENVIRONMENTs, LOADs, or PRODUCTs. Within each of these UDB sectors, each dataset is CATALOGed via a unique accession number (UDB#). When transferring data between foreground memory (the activity database or ADB) and a UDB, the target location must be specified by the name of the UDB sector and the accession number within

the sector. For example, to STORE the current pattern of chemical loadings: STORE LOAD 7. Similarly, to retrieve or RECALL data from a UDB into the ADB for use in an analysis, one could enter: RECALL LOAD 7.

VAPR

VAPoR pressure (chemical) Units: Torr

Used to compute Henry's law constant when HENRY datum is zero (0) but VAPR is non-zero:

$$\text{HENRY} = \frac{\text{VAPR} / 760.}{\text{SOL} / \text{MWT}}$$

If the associated molar heat of vaporization (EVPR) is non-zero, VAPR is taken as the base-10 logarithm of the pre-exponential factor in an exponential function describing vapor pressure as a function of temperature (TCEL).

VOL

VOLume (segment) Units: m^3

Total environmental volume of ecosystem segments.

WIDTH

WIDTH (segment) Units: m

Average bank-to-bank distance -- for computing volume, area, depth of lotic systems described via length, width, and cross-sectional areas.

WIND

WINDspeed (segment, month) Units: m/second

Average wind velocity at a reference height of ten centimeters above the water surface. Parameter is used to compute a piston velocity for water vapor (Liss 1973, Deep-Sea Research 20:221) in the 2-resistance treatment of volatilization losses.

XSA

Cross-sectional (XS) Area (segment) Units: m^2

Area of waterbody in section along advective flowpath.

XSTUR

XSection for TURbulent dispersion (path) Units: m^2

XSTUR is cross-sectional area of a dispersive exchange interface at the boundary between segments JTURB(p) and ITURB(p). The matching (same "p" subscript) members of JTURB, ITURB, CHARL, DSP, and XSTUR collectively

define a dispersive transport pathway. The exchange constant E(p) is computed as:

E(p) (m^3/hour) = DSP(p) XSTUR(p) / CHARL(p)

See also: CHARL, DSP, ITURB, JTURB

YEAR1

YEAR 1 Units: n/a

Starting year for mode 3 simulation (e.g., 1985).

YIELD

YIELD of product (path) Units: mole/mole

YIELD(p) is the product yield from the transformation pathway "p" with dimensions mole of transformation product TPROD(p) produced per mole of parent compound CHPAR(p) reacted (dimensionless).

See also: CHPAR, EAYLD, NPROC, RFORM, TPROD

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